9-30-06

ACCESS DB # 200417

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SEP - 6 2006

(STIC)

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner # : 59193 Date: 9/1

Art Unit: 1624 Phone Number: 2- 0663 Serial Number: 10608689

Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): (PAPER) DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following: ME

Title of Invention: _____

Inventors (please provide full names): _____

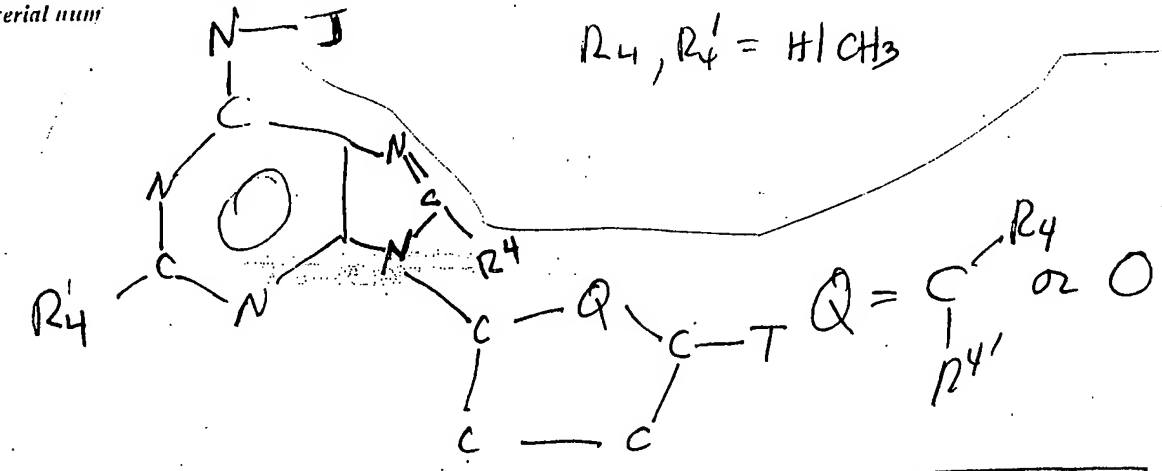
_____

Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial num*



$R_4, R_4' = H \mid CH_3$

$T = C - A - Hal$

A = Bond or linker of 1-20 atoms, each = C or O or Ring-N

#1 of 2

↑ cannot be $C^{Q''}$ or C-in-a-heterocyclic ring or C-in-a-phenyl ring

$Q'' = O \mid S \mid N$

J = C (Ring or chain, but J ≠ [O]). If Q=O, then (claim)

J ≠ Cycloalkyl-$(Hal)_{0-6}$ or alkyl-$(OH)_{0-6}$

Recheck CII and note provisos

In addition, if Q=O and T = CH_2 Hal, then J ≠ alkyl or C_n-C=C (n = 0-10)

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 11:48:08 ON 08 SEP 2006

=> d his

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                ACT BER689/A
L1              STR
L2              STR
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L4           180 SEA FILE=REGISTRY SUB=L3 SSS FUL L2
L5              STR L1
L6            50 S L5

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L7             1 S US20040127434/PN
                SEL RN

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L8            36 S E1-E36
L9              STR
L10            0 S L9
L11             STR L9
L12           46 S L11
L13             STR L11
L14           50 S L13
L15       131651 S L13 FUL
L16           24 S L8 AND L15
L17             STR L11
L18           23 S L17 SAM  SUB=L15
L19          479 S L17 FUL  SUB=L15
L20           12 S L19 AND L16
L21          278 S L19 NOT 1-100/P
L22           12 S L16 NOT L20
L23             STR L17
L24            2 S L23 SAM  SUB=L15
L25           49 S L23 FUL  SUB=L15
L26          229 S L21 NOT L25

     FILE 'HCAPLUS' ENTERED AT 11:32:20 ON 08 SEP 2006
L27           18 S L25
L28          126 S L26

     FILE 'REGISTRY' ENTERED AT 11:33:16 ON 08 SEP 2006
L29             STR
L30            7 S (L17 NOT L29) SAM  SUB=L15
L31          170 S (L17 NOT L29) FUL  SUB=L15
L32          128 S L31 NOT L25
L33           86 S L32 NOT 1-100/P
L34             STR L17
L35            0 S (L34 NOT L29) SAM  SUB=L15
L36           14 S (L34 NOT L29) FUL  SUB=L15

     FILE 'HCAPLUS' ENTERED AT 11:44:30 ON 08 SEP 2006
L37           31 S L33
L38            4 S L36
L39           22 S L27 OR L38
L40           23 S L37 NOT L39
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```
=> d que l39
L13              STR
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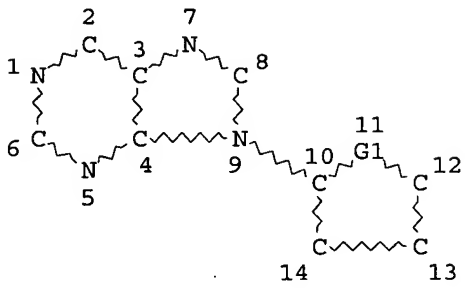

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VAR G1=O/C
NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
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L23              STR
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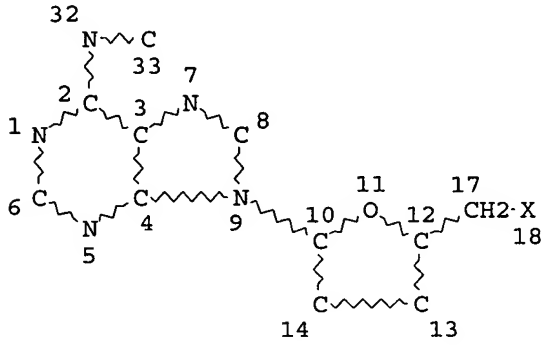

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  19

STEREO ATTRIBUTES: NONE
L25           49 SEA FILE=REGISTRY SUB=L15 SSS FUL L23
L27           18 SEA FILE=HCAPLUS ABB=ON  L25
L29              STR
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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
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DEFAULT ECLEVEL IS LIMITED

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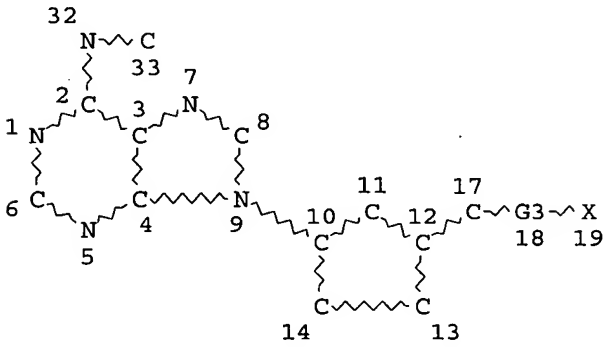
NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE
L34 STR



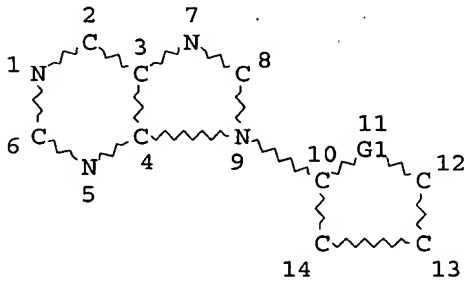
A @20

REP G3=(0-20) 20
NODE ATTRIBUTES:
NSPEC IS RC AT 20
NSPEC IS RC AT 33
CONNECT IS E2 RC AT 17
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L36 14 SEA FILE=REGISTRY SUB=L15 SSS FUL (L34 NOT L29)
L38 4 SEA FILE=HCAPLUS ABB=ON L36
L39 22 SEA FILE=HCAPLUS ABB=ON L27 OR L38

=> d que l40
L13 STR



VAR G1=O/C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
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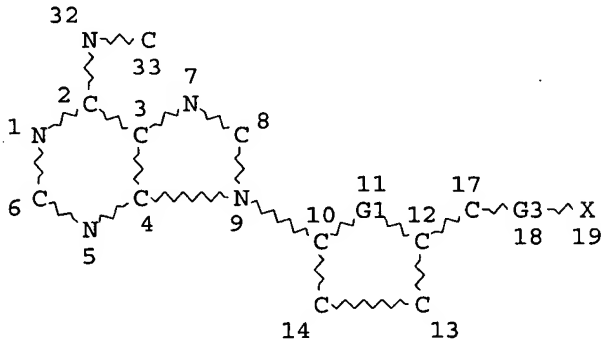
L17 STR

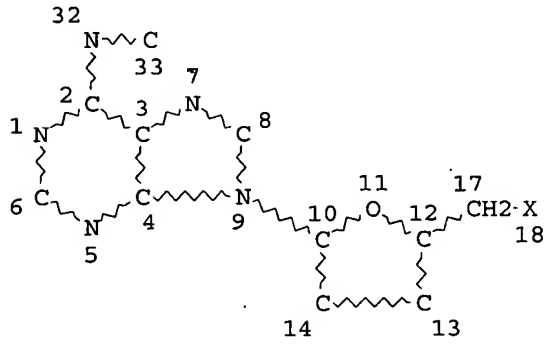


A @20

VAR G1=O/C
REP G3=(0-20) 20
NODE ATTRIBUTES:
NSPEC IS RC AT 20
NSPEC IS RC AT 33
CONNECT IS E2 RC AT 17
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L23 STR



A 20

NODE ATTRIBUTES:
NSPEC IS RC AT 20
NSPEC IS R AT 33
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

```
L25           49 SEA FILE=REGISTRY SUB=L15 SSS FUL L23
L27           18 SEA FILE=HCAPLUS ABB=ON  L25
L29              STR

C===O
1   2

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   2

STEREO ATTRIBUTES: NONE
L31          170 SEA FILE=REGISTRY SUB=L15 SSS FUL (L17 NOT L29)
L32          128 SEA FILE=REGISTRY ABB=ON  L31 NOT L25
L33           86 SEA FILE=REGISTRY ABB=ON  L32 NOT 1-100/P
L34              STR
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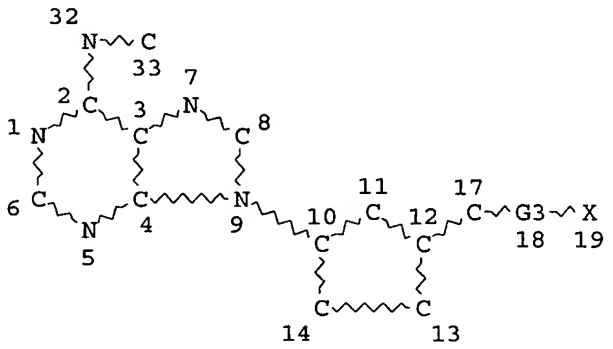

A @20

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REP G3=(0-20) 20
NODE ATTRIBUTES:
NSPEC   IS RC     AT  20
NSPEC   IS RC     AT  33
CONNECT IS E2  RC AT  17
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE
L36           14 SEA FILE=REGISTRY SUB=L15 SSS FUL (L34 NOT L29)
L37           31 SEA FILE=HCAPLUS ABB=ON  L33
L38            4 SEA FILE=HCAPLUS ABB=ON  L36
L39           22 SEA FILE=HCAPLUS ABB=ON  L27 OR L38
L40           23 SEA FILE=HCAPLUS ABB=ON  L37 NOT L39


=> fil hcap
FILE 'HCAPLUS' ENTERED AT 11:48:26 ON 08 SEP 2006


=> d 139 1-22 ibib abs hitstr hitind
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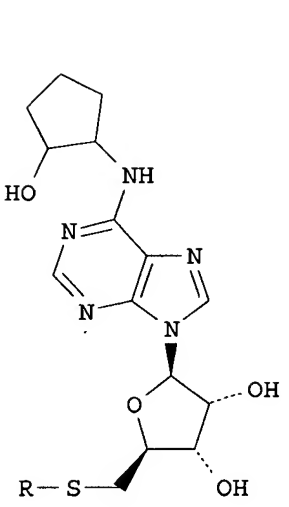
L39 ANSWER 1 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:213018 HCAPLUS
DOCUMENT NUMBER: 144:274496
TITLE: Process for the preparation of thionucleoside analog via condensation of 5'-deoxychloro nucleosides with thiols as A1 adenosine receptor agonists
INVENTOR(S): Zablocki, Jeff; Elzein, Elfatih; Organ, Michael G.; Bilokin, Yaroslav; Mayer, Stanislas; Disanti, Anthony; Miller, Scott A.; Kernast, Peter A.
PATENT ASSIGNEE(S): CV Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006026651	A1	20060309	WO 2005-US30938	2005 0830
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2006052330	A1	20060309	US 2005-214706	2005 0829

PRIORITY APPLN. INFO.:	US 2004-606083P	P	2004 0830
	US 2004-622076P	P	2004 1026

OTHER SOURCE(S): MARPAT 144:274496
GI



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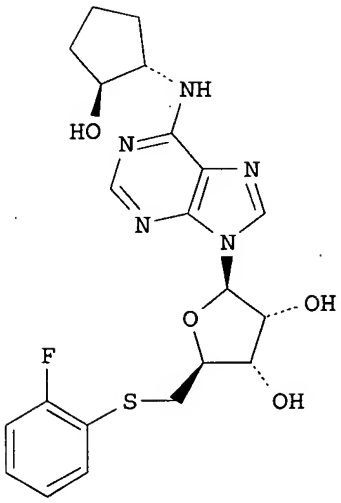


II

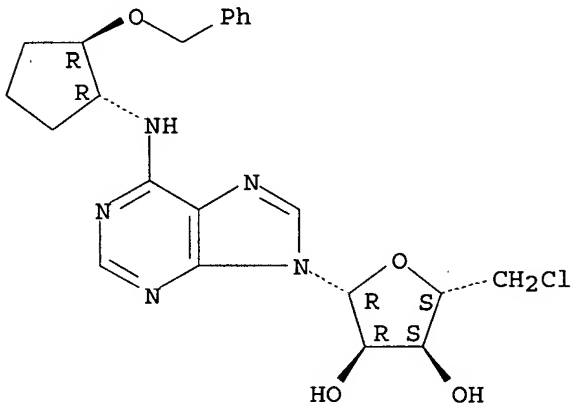
AB A process for the large scale synthesis of thionucleoside analogs, I, wherein R is optionally substituted Ph, are useful as partial and full A1 adenosine receptor agonists in the treatment of various diseases such as tachycardia and atrial flutter, angina, and myocardial infarction. The method consists of condensation of (4S,2R,3R,5R)-2-(6-chloropurin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol with a (2-hydroxy)-protected cyclopentylamine, followed by thionyl chloride addition, then protecting group removal, derivatizing the thiol group and final deprotection. Thus, II was prepared and tested in DDT1, [35S]GTPγS, and cAMP cell binding assays (no data).

IT **872693-39-5P 872693-40-8P 872693-41-9P**
872693-42-0P 872853-92-4P
(process for the preparation of thionucleoside analogs for potential use as A1 adenosine receptor agonists)

RN 872693-39-5 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-[(1R,2R)-2-(phenylmethoxy)cyclopentyl]- (9CI) (CA INDEX NAME)

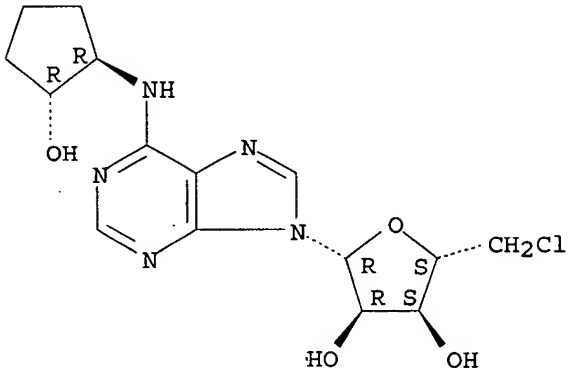
Absolute stereochemistry.



RN 872693-40-8 HCAPLUS

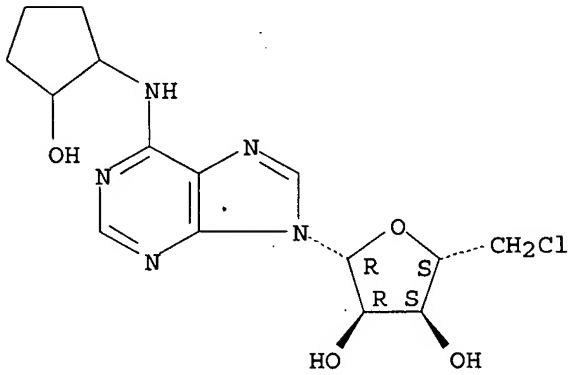
CN Adenosine, 5'-chloro-5'-deoxy-N-[(1R,2R)-2-hydroxycyclopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 872693-41-9 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(2-hydroxycyclopentyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 872693-42-0 HCAPLUS
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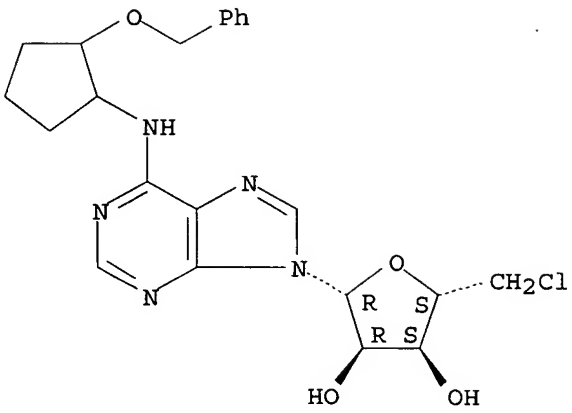
Absolute stereochemistry.



RN 872853-92-4 HCAPLUS
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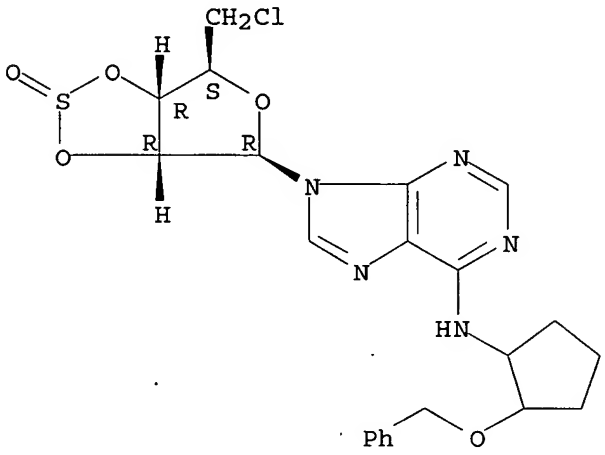
Absolute stereochemistry.



IC ICM C07H019-16
ICS A61K031-7008
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT 872693-38-4P **872693-39-5P 872693-40-8P**
872693-41-9P 872693-42-0P 872693-43-1P
872853-92-4P
(process for the preparation of thionucleoside analogs for potential use as A1 adenosine receptor agonists)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:36872 HCAPLUS
DOCUMENT NUMBER: 144:129188
TITLE: Process for the preparation of thionucleoside analog via condensation of 5'-deoxychloro nucleosides with thiols as A1 adenosine

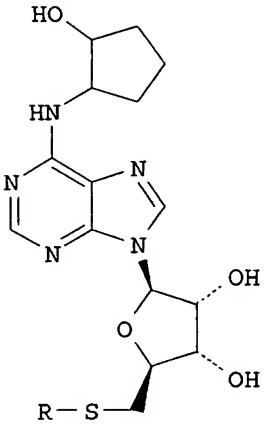
receptor agonists
INVENTOR(S): Elzein, Elfatih; Zablocki, Jeff
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 21 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006009417	A1	20060112	US 2005-173416	20050630
WO 2006017052	A1	20060216	WO 2005-US23628	20050630

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-587100P P 20040712

OTHER SOURCE(S): MARPAT 144:129188
GI



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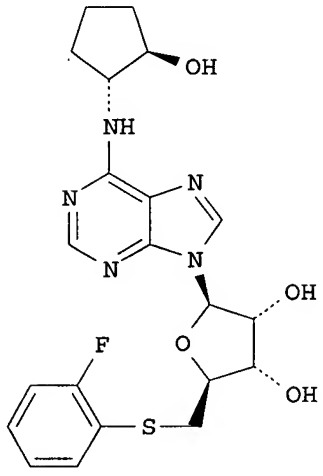


II

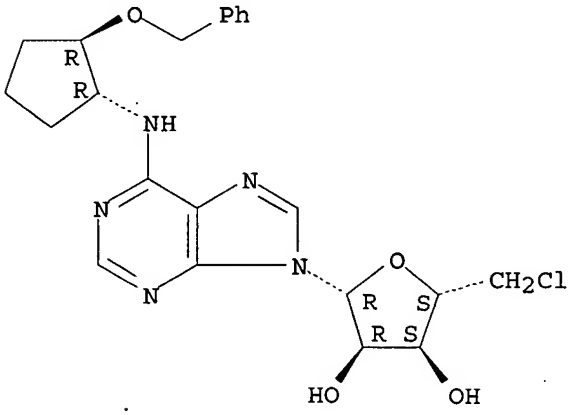
AB A process for the large scale synthesis of thionucleoside analogs, I, wherein R is optionally substituted Ph, are useful as partial and full A1 adenosine receptor agonists in the treatment of various diseases such as tachycardia and atrial flutter, angina, and myocardial infarction. Thus, II was prepared and tested in DDT1, [35S]GTPγS, and cAMP cell binding assays (no data). The method consists of condensation of (4S,2R,3R,5R)-2-(6-chloropurin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol with a (2-hydroxy)-protected cyclopentylamine, followed by thionyl chloride addition, then protecting group removal, derivatizing the thiol group and final deprotection.

IT **872693-39-5P 872693-40-8P 872693-41-9P 872693-42-0P 872853-92-4P**
(process for the preparation of thionucleoside analogs for potential use as A1 adenosine receptor agonists)

RN 872693-39-5 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-[(1R,2R)-2-(phenylmethoxy)cyclopentyl]- (9CI) (CA INDEX NAME)

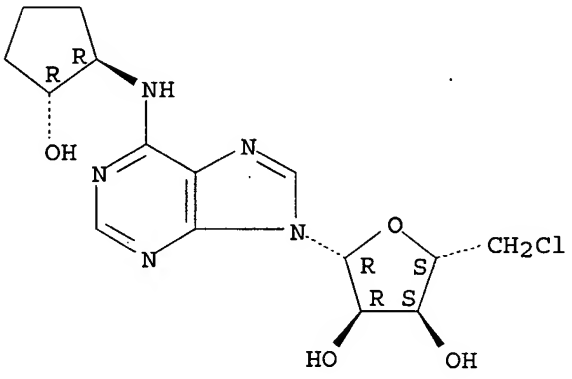
Absolute stereochemistry.



RN 872693-40-8 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-[(1R,2R)-2-hydroxycyclopentyl]- (9CI) (CA INDEX NAME)

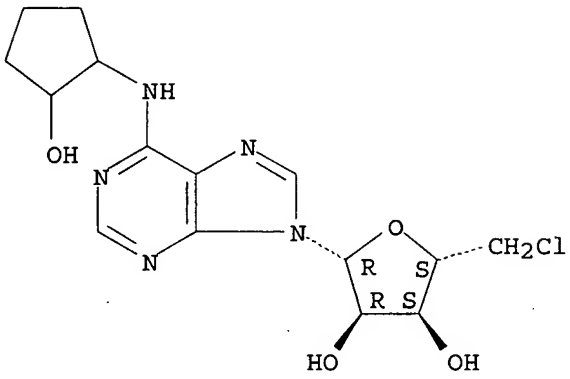
Absolute stereochemistry.



RN 872693-41-9 HCAPLUS

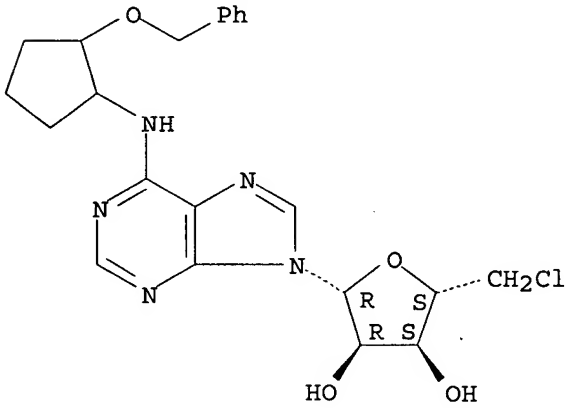
CN Adenosine, 5'-chloro-5'-deoxy-N-(2-hydroxycyclopentyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



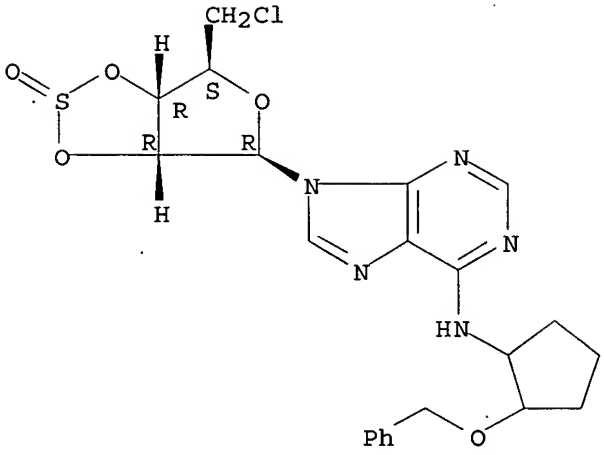
RN 872693-42-0 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-[2-(phenylmethoxy)cyclopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 872853-92-4 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-[2-(phenylmethoxy)cyclopentyl]-, cyclic 2',3'-sulfite (9CI) (CA INDEX NAME)

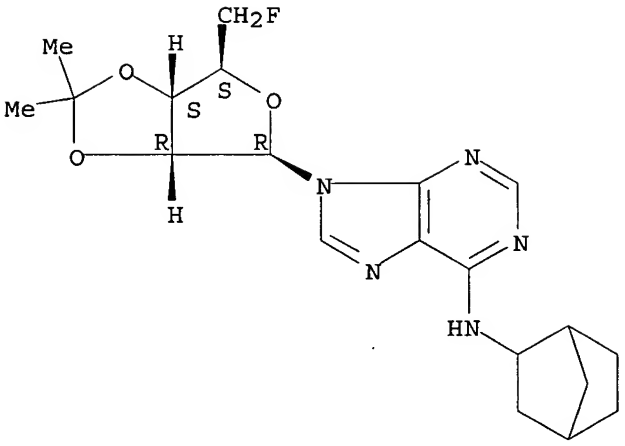
Absolute stereochemistry.



INCL 514046000; 536027300
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT 872693-38-4P **872693-39-5P 872693-40-8P**
872693-41-9P 872693-42-0P 872693-43-1P
872853-92-4P
(process for the preparation of thionucleoside analogs for potential use as A1 adenosine receptor agonists)

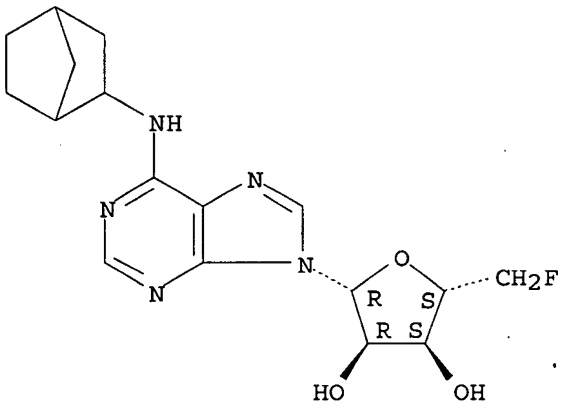
L39 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:544591 HCAPLUS
DOCUMENT NUMBER: 143:230124
TITLE: An improved synthesis of 5'-fluoro-5'-deoxyadenosines
AUTHOR(S): Ashton, Trent D.; Scammells, Peter J.
CORPORATE SOURCE: Department of Medicinal Chemistry, Victorian College of Pharmacy, Monash University, Parkville, 3052, Australia
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(14), 3361-3363
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:230124
AB Synthesis of 5'-fluoro-5'-deoxyadenosine (5'-FDA) and structurally similar compds. is generally a poor yielding process. This is attributed to the instability of the selected synthetic intermediates. Herein, we report a general synthesis of 5'-fluoro-5'-deoxy-N6-substituted adenosines including a high yielding access to 5'-FDA.
IT **862844-64-2P**
(improved synthesis of 5'-fluoro-5'-deoxy-N6-substituted adenosines)
RN 862844-64-2 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-deoxy-5'-fluoro-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **224045-32-3P**
(improved synthesis of 5'-fluoro-5'-deoxy-N6-substituted adenosines)
RN 224045-32-3 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-deoxy-5'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-9 (Carbohydrates)
IT 449205-33-8P 862672-09-1P 862672-10-4P **862844-64-2P**
(improved synthesis of 5'-fluoro-5'-deoxy-N6-substituted adenosines)
IT 731-98-6P **224045-32-3P**
(improved synthesis of 5'-fluoro-5'-deoxy-N6-substituted adenosines)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:835882 HCAPLUS
DOCUMENT NUMBER: 142:273338
TITLE: Interaction of nucleoside analogues with nucleoside transporters in rat brain

endothelial cells

AUTHOR(S): Chishty, Mansoor; Begley, David J.; Abbott, N. Joan; Reichel, Andreas

CORPORATE SOURCE: Blood-Brain Barrier Research Group, Centre for Neuroscience Research, GKT School of Biomedical Sciences, King's College London, London, SE1 1UL, UK

SOURCE: Journal of Drug Targeting (2004), 12(5), 265-272
CODEN: JDTAEH; ISSN: 1061-186X

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

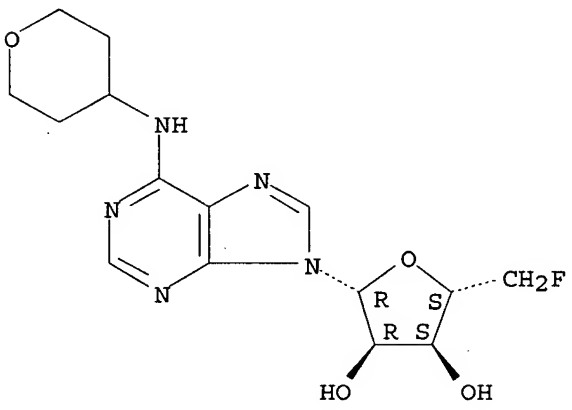
AB A number of nucleoside analogs, consisting of antiviral compds. and agents designed as adenosine A1 receptor agonists, were examined for nucleoside transporter affinity using an in vitro model of the blood-brain barrier (BBB), the rat brain endothelial cell line, RBE4. Structure-activity relationships (SAR) were also performed to identify the key structural requirements for transporter recognition and the suitability of these systems for carrier-mediated strategies to deliver therapeutics across the BBB. Adenosine receptor agonists did not show transport affinity for concentrative nucleoside carriers, but exhibited affinity for equilibrative systems (Ki = 10.8-97.9 μM) within the range of Kms for natural substrates. However, none of the antiviral compds. tested in this study showed affinity for either class of nucleoside transporter. SAR studies suggest that the hydroxyl group located at the 3'-position of the ribose moiety is an essential requirement for transporter recognition. This may explain the inability of nucleoside derived anti-viral compds. to use these systems despite the significant structural homol. with naturally occurring nucleosides. Sites have also been identified which accommodate structural addns. with retention of carrier affinity, suggesting that compds. which fail to penetrate the BBB could be attached to these sites for carrier-mediated delivery using a prodrug strategy.

IT **223774-67-2**, GR 242468 **223774-74-1**, GR 395849
(interaction of nucleoside analogs with nucleoside transporters in rat brain endothelial cells)

RN 223774-67-2 HCAPLUS

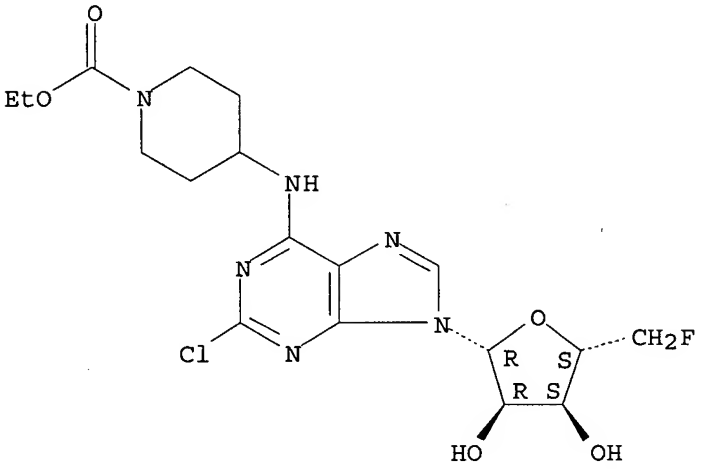
CN Adenosine, 5'-deoxy-5'-fluoro-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 223774-74-1 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[2-chloro-9-(5-deoxy-5-fluoro-β-D-ribofuranosyl)-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-3 (Pharmacology)
IT 50-89-5, Thymidine, biological studies 58-61-7, Adenosine, biological studies 65-46-3, Cytidine 3056-17-5, Stavudine 23589-16-4, CCI 4019 30516-87-1, Zidovudine 110299-05-3, GR 56072X 119644-22-3, GW 274666X 120465-16-9, GR 56071X 124555-18-6, GR 79236X 134678-17-4, Lamivudine 222159-14-0, GR 666683X 223756-75-0, GR 150185 **223774-67-2**, GR 242468 **223774-74-1**, GR 395849
(interaction of nucleoside analogs with nucleoside transporters in rat brain endothelial cells)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:611329 HCAPLUS
DOCUMENT NUMBER: 142:261724
TITLE: First no-carrier-added radio-selenation of an adenosine-A1 receptor ligand
AUTHOR(S): Blum, Till; Ermert, Johannes; Wutz, Walter; Bier, Dirk; Coenen, Heinz H.
CORPORATE SOURCE: Forschungszentrum Juelich GmbH, Institut fuer Nuklearchemie, Juelich, D-52425, Germany
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2004), 47(7), 415-427
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:261724
AB The precursor synthesis and the no-carrier-added (n.c.a.) radiosynthesis of the adenosine-A1 receptor ligand 5'-(methyl[75Se]seleno)-N6-cyclopentyladenosine [75Se] are

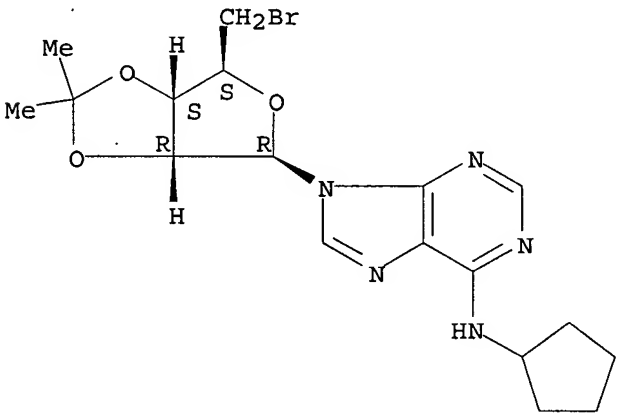
described in this report. A method was developed starting from elemental n.c.a. selenium-75, followed by a three-step polymer-supported radio-selenation and deprotection which gave the radio-ligand with a radiochem. yield of 30%, a radiochem. purity of > 99% and a specific radioactivity of > 300 GBq/mmol (8 Ci/mmol). Preparation time was 40 min. The nonradioactive compound 5'-(methyl-seleno)-N6-cyclopentyladenosine was pharmacol. evaluated in vitro and showed high affinity and selectivity for the adenosine-A1 receptor. These preliminary results suggest that this compound could be a useful radioligand for the non-invasive imaging of the brain adenosine-A1 receptors using positron emission tomog. (PET) when labeled with the positron emitter selenium-73 (half-life: 7.1 h).

IT **117325-48-1P**
(preparation and radio-selenation of an adenosine-A1 receptor ligand)

RN 117325-48-1 HCAPLUS

CN Adenosine, 5'-bromo-N-cyclopentyl-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-9 (Carbohydrates)
Section cross-reference(s): 6, 74

IT 9003-53-6DP, Polystyrene, aminomethylated reaction products with cyclohexylaminoselenoaldehyde derivs. 41552-82-3P 103626-58-0P **117325-48-1P** 846552-43-0P 846552-44-1DP, aminomethylated polystyrene resin bound 846552-46-3DP, aminomethylated polystyrene resin bound 846552-47-4P
(preparation and radio-selenation of an adenosine-A1 receptor ligand)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:5177 HCAPLUS

DOCUMENT NUMBER: 140:42425

TITLE: Preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes

INVENTOR(S): Bigot, Antony; Stengelin, Siegfried; Jaehne, Gerhard; Herling, Andreas; Mueller, Guenter;

Hock, Franz Jakob; Myers, Michael R.
PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1375508	A1	20040102	EP 2002-14324	20020627
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CA 2490253	AA	20040108	CA 2003-2490253	20030626
WO 2004003002	A1	20040108	WO 2003-EP6749	20030626
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003280141	A1	20040119	AU 2003-280141	20030626
BR 2003012428	A	20050426	BR 2003-12428	20030626
EP 1527083	A1	20050504	EP 2003-740352	20030626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671728	A	20050921	CN 2003-817966	20030626
JP 2006501178	T2	20060112	JP 2004-516688	20030626
US 2004127434	A1	20040701	US 2003-608689	20030627
NO 2005000398	A	20050125	NO 2005-398	20050125

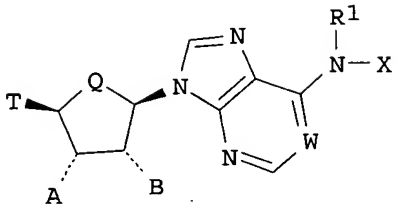
PRIORITY APPLN. INFO.: EP 2002-14324 A

2002
0627

US 2002-434164P P
2002
1217

WO 2003-EP6749 W
2003
0626

OTHER SOURCE(S): MARPAT 140:42425
GI



I

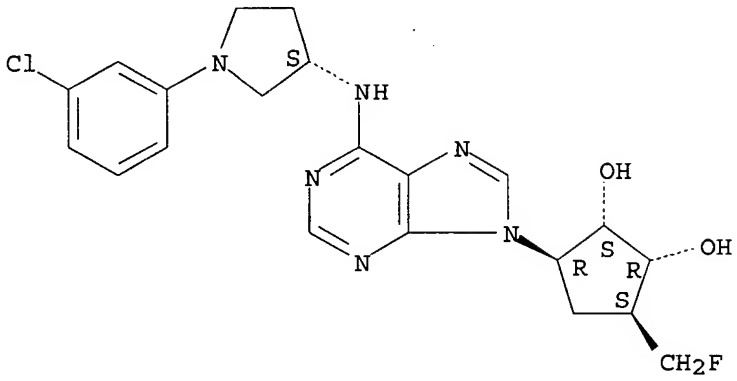
AB Adenosine analogs I, wherein W is N, NO, CH; Q is CH2, O; R1 is alkyl, allyl, 2-methylallyl, 2-butenyl, cycloalkyl; X is heterocycle; T is cycloalkyl, aryl-(alkylene)-, heterocyclyl-(alkylene), which residues are monosubstituted by halogen or OR2, halogen, pseudo-halogen, mercapto, NH2, nitro, hydroxy, unsubstituted and at least monosubstituted alkyl, alkoxy, (alkyl)amino, (alkyl)thio, aryl and heterocyclyl; R2 is alkyl substituted by at least one halogen; A and B are independently H, alkyl, hydroxy-(alkylene)-, alkoxy-(alkylene)-, or OR'; R' is hydrogen, alkyl, aryl-(alkylene)-, (alkyl)-CO, carbo-alkoxy, aryl-(alkylene)-CO-, and aryl-O-CO-; were prepared for the treatment of insulin resistance syndrome and diabetes. These compds. are useful for the manufacture of a medicament for the treatment of insulin resistance, type 2 diabetes, metabolic syndrome, lipid disorders or cardiovascular disease or for providing an anti-lipolytic effect. Thus, (1R,2S,3R,5S)-3-{6-[1-(3-chloro-phenyl-1-yl)-pyrrolidin-3(S)-ylamino]-purin-9-yl}-5-fluoromethylcyclopentane-1,2-diol was prepared and used in vitro or the treatment of insulin resistance syndrome and diabetes. Measurement of insulin sensitivity in conscious insulin resistant Zucker fatty rats or Zucker diabetic fatty (ZDF) rats is reported. Effect of title nucleosides on contractile force and heart rate, is reported.

IT **636600-26-5P 636600-28-7P 636600-31-2P**
636600-34-5P 636600-35-6P 636600-36-7P
636600-37-8P 636600-38-9P 636600-39-0P
636600-40-3P
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)

RN 636600-26-5 HCAPLUS

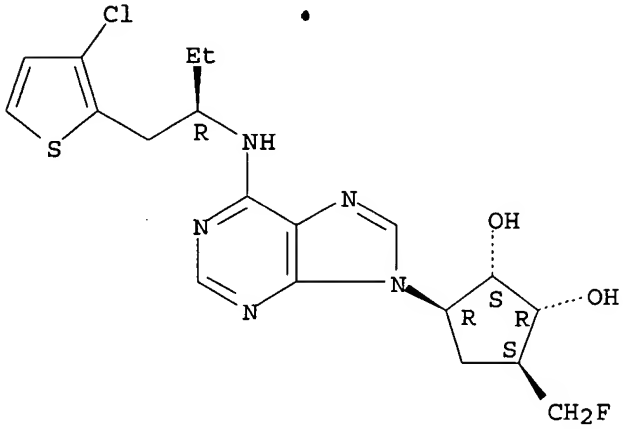
CN 1,2-Cyclopentanediol, 3-[6-[[(3S)-1-(3-chlorophenyl)-3-pyrrolidinyl]amino]-9H-purin-9-yl]-5-(fluoromethyl)-, (1R,2S,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



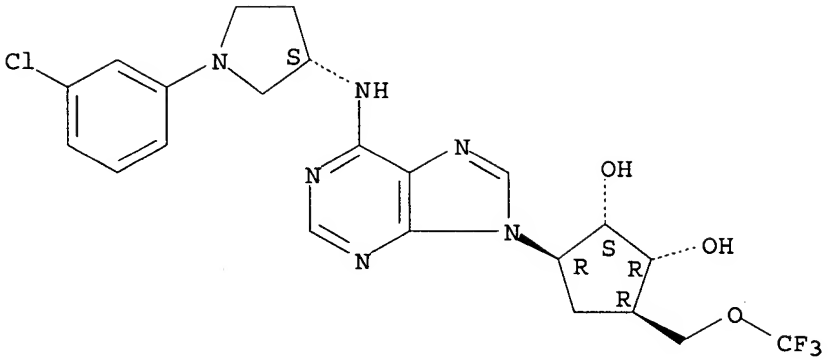
RN 636600-28-7 HCAPLUS
CN 1,2-Cyclopentanediol, 3-[6-[[(1R)-1-[(3-chloro-2-thienyl)methyl]propyl]amino]-9H-purin-9-yl]-5-(fluoromethyl)-, (1R,2S,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



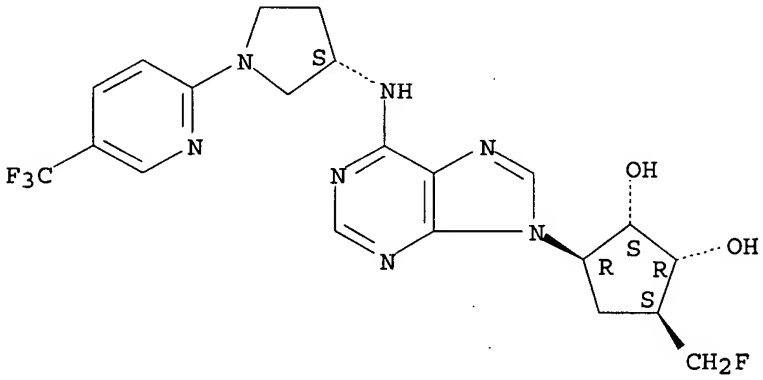
RN 636600-31-2 HCAPLUS
CN 1,2-Cyclopentanediol, 3-[6-[[(3S)-1-(3-chlorophenyl)-3-pyrrolidinyl]amino]-9H-purin-9-yl]-5-[(trifluoromethoxy)methyl]-, (1R,2S,3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



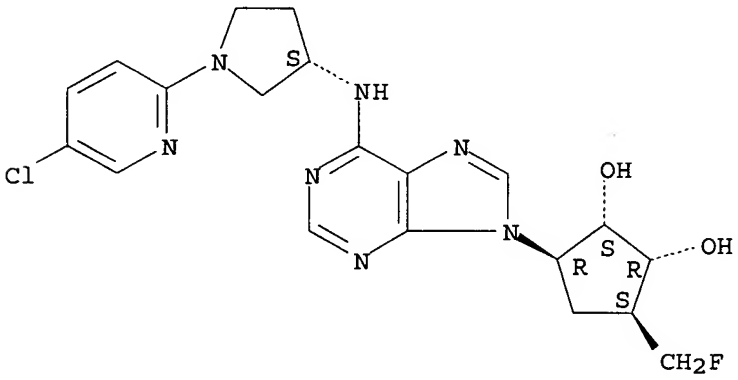
RN 636600-34-5 HCAPLUS
CN 1,2-Cyclopentanediol, 3-(fluoromethyl)-5-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



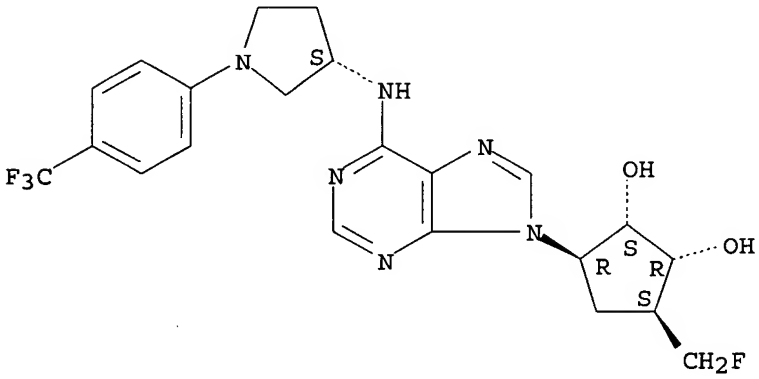
RN 636600-35-6 HCAPLUS
CN 1,2-Cyclopentanediol, 3-[6-[[(3S)-1-(5-chloro-2-pyridinyl)-3-pyrrolidinyl]amino]-9H-purin-9-yl]-5-(fluoromethyl)-, (1R,2S,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



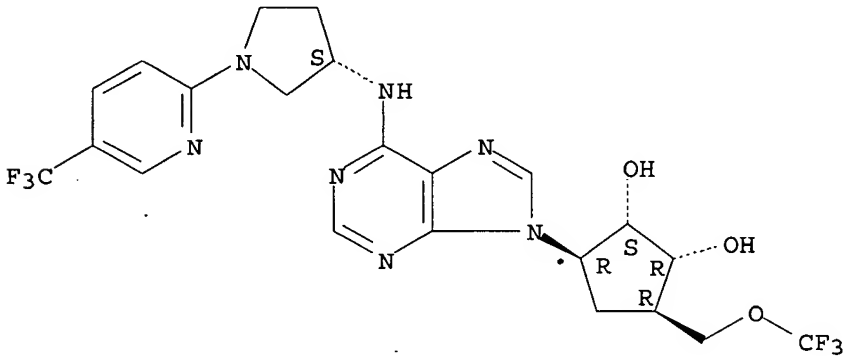
RN 636600-36-7 HCAPLUS
CN 1,2-Cyclopentanediol, 3-(fluoromethyl)-5-[6-[[(3S)-1-[4-(trifluoromethyl)phenyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



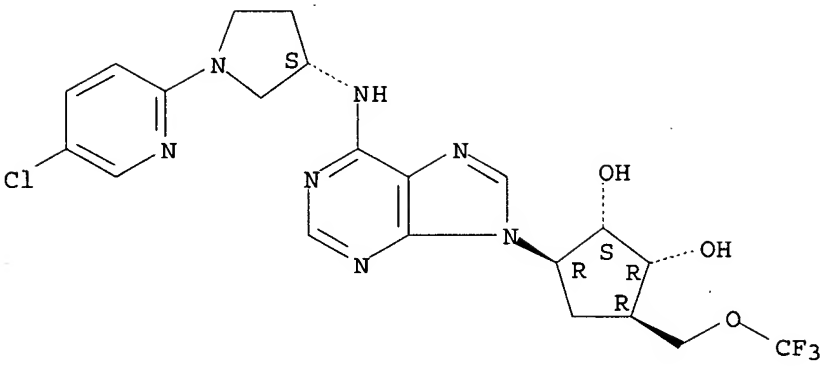
RN 636600-37-8 HCAPLUS
CN 1,2-Cyclopentanediol, 3-[(trifluoromethoxy)methyl]-5-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



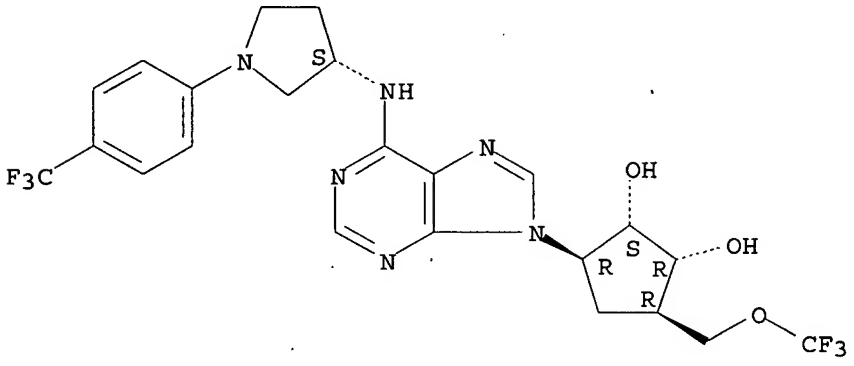
RN 636600-38-9 HCAPLUS
CN 1,2-Cyclopentanediol, 3-[6-[[(3S)-1-(5-chloro-2-pyridinyl)-3-pyrrolidinyl]amino]-9H-purin-9-yl]-5-[(trifluoromethoxy)methyl]-, (1R,2S,3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



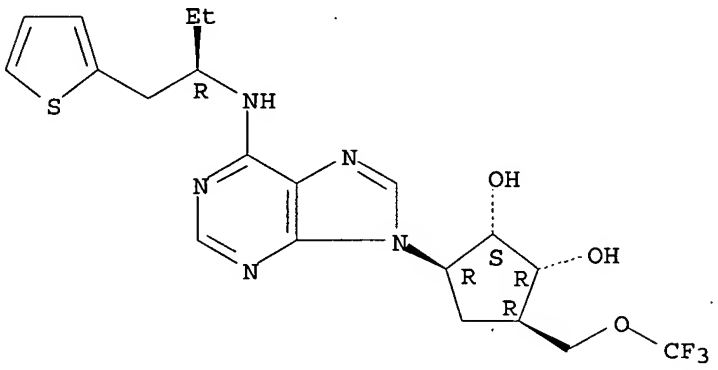
RN 636600-39-0 HCAPLUS
CN 1,2-Cyclopentanediol, 3-[(trifluoromethoxy)methyl]-5-[6-[[(3S)-1-[4-(trifluoromethyl)phenyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



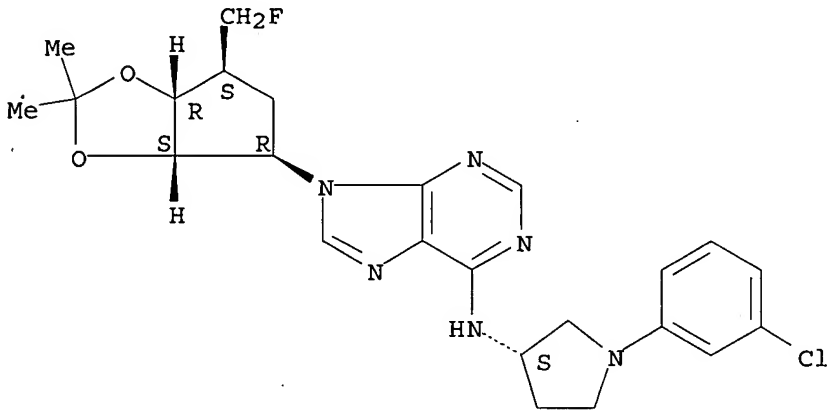
RN 636600-40-3 HCAPLUS
CN 1,2-Cyclopentanediol, 3-[6-[[(1R)-1-(2-thienylmethyl)propyl]amino]-9H-purin-9-yl]-5-[(trifluoromethoxy)methyl]-, (1R,2S,3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



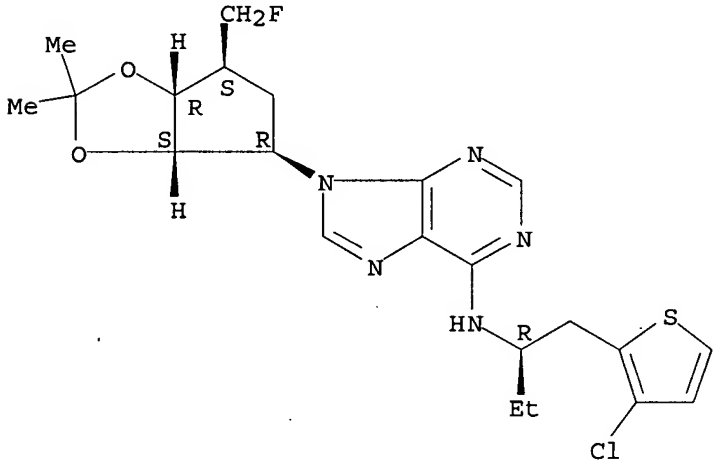
IT **636600-27-6P 636600-29-8P**
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)
RN 636600-27-6 HCAPLUS
CN 9H-Purin-6-amine, N-[(3S)-1-(3-chlorophenyl)-3-pyrrolidinyl]-9-[(3aS,4R,6S,6aR)-6-(fluoromethyl)tetrahydro-2,2-dimethyl-4H-cyclopenta-1,3-dioxol-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 636600-29-8 HCAPLUS
CN 9H-Purin-6-amine, N-[(1R)-1-[(3-chloro-2-thienyl)methyl]propyl]-9-[(3aS,4R,6S,6aR)-6-(fluoromethyl)tetrahydro-2,2-dimethyl-4H-cyclopenta-1,3-dioxol-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-167
ICS A61K031-70
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT **636600-26-5P 636600-28-7P 636600-31-2P**
636600-34-5P 636600-35-6P 636600-36-7P
636600-37-8P 636600-38-9P 636600-39-0P

636600-40-3P 636600-41-4P 636600-42-5P 636600-43-6P
636600-44-7P 636600-45-8P 636600-46-9P 636600-47-0P
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)
IT 636600-20-9P 636600-21-0P 636600-22-1P 636600-23-2P
636600-25-4P **636600-27-6P 636600-29-8P**
636600-30-1P 636600-33-4P
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:472502 HCAPLUS
DOCUMENT NUMBER: 135:66249
TITLE: Formulations of adenosine A1 receptor agonists as analgesics
INVENTOR(S): Bountra, Charanjit; Clayton, Nicholas Maughan; Naylor, Alan
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001045715	A2	20010628	WO 2000-GB4885	2000 1219
WO 2001045715	A3	20020314		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1248632	A2	20021016	EP 2000-985629	2000 1219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003518068	T2	20030603	JP 2001-546654	2000 1219
US 2003004126	A1	20030102	US 2002-168189	2002 0618
PRIORITY APPLN. INFO.:			GB 1999-30071 A	1999 1220

WO 2000-GB4885 W
2000
1219

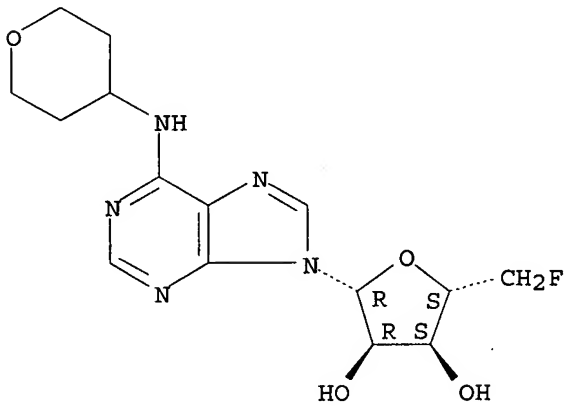
AB A method of treating conditions associated with pain and alleviating the symptoms associated with it comprises administering to a mammal, an adenosine A1 agonist or a physiol. acceptable salt or a solvate and an opioid. The present invention also provides pharmaceutical formulations and patient packs comprising the combinations. 5'-Deoxy-5'-fluoro-N-(tetrahydropyran-4-yl)adenosine and administered orally to rats and morphine was administered s.c. to the same rats. The compds. inhibited carrageenan-induced edema and allodynia.

IT **223774-67-2**
(formulations of adenosine A1 receptor agonists as analgesics)

RN 223774-67-2 HCAPLUS

CN Adenosine, 5'-deoxy-5'-fluoro-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K031-7076
ICS A61K031-52; A61K031-485; A61P029-00; A61K031-7076; A61K031-485

CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1, 33

IT 57-27-2, Morphine, biological studies 57-42-1, Pethidine 58-61-7, Adenosine, biological studies 76-42-6, Oxycodone 76-57-3, Codeine 76-99-3, Methadone 77-07-6, Levorphanol 125-28-0, Dihydrocodeine 359-83-1, Pentazocine 437-38-7, Fentanyl 469-62-5, Dextropropoxyphene 561-27-3, Diamorphine 52485-79-7, Buprenorphine 71195-58-9, Alfentanil 124555-18-6 **223774-67-2** 346425-37-4
(formulations of adenosine A1 receptor agonists as analgesics)

L39 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:325950 HCAPLUS
DOCUMENT NUMBER: 130:338350
TITLE: Preparation of deoxyfluoro nucleosides as adenosine A1 receptors
INVENTOR(S): Cousins, Richard Peter Charles; Cox, Brian; Eldred, Colin David; Pennell, Andrew Michael Kenneth

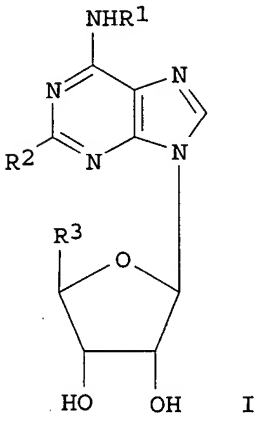
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9924449	A2	19990520	WO 1998-EP7021	1998 1106
WO 9924449	A3	19990819		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
ZA 9810125	A	20000505	ZA 1998-10125	1998 1105
CA 2309200	AA	19990520	CA 1998-2309200	1998 1106
AU 9920483	A1	19990531	AU 1999-20483	1998 1106
EP 1030857	A2	20000830	EP 1998-965151	1998 1106
EP 1030857	B1	20040818		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9813976	A	20000926	BR 1998-13976	1998 1106
TR 200002131	T2	20010122	TR 2000-200002131	1998 1106
EE 200000285	A	20010815	EE 2000-285	1998 1106
JP 2001522857	T2	20011120	JP 2000-520457	1998 1106
AT 273990	E	20040915	AT 1998-965151	1998 1106
EP 1457495	A1	20040915	EP 2004-76482	1998 1106
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
ES 2222621	T3	20050201	ES 1998-965151	

					1998 1106
NO 2000002361	A	20000705	NO 2000-2361		2000 0505
HR 2000000275	A1	20001231	HR 2000-275		2000 0508
US 6455510	B1	20020924	US 2000-530573		2000 0615
PRIORITY APPLN. INFO.:			GB 1997-23589	A	1997 1108
			EP 1998-965151	A3	1998 1106
			WO 1998-EP7021	W	1998 1106

OTHER SOURCE(S): MARPAT 130:338350

GI



I

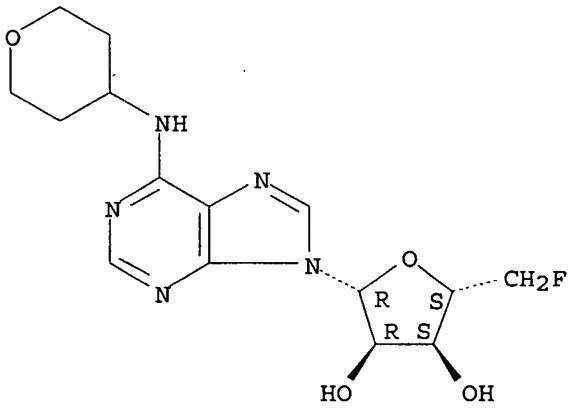
AB Deoxyfluoro nucleosides I which are agonists at the adenosine A1 receptor wherein R1 represents cycloalkyl, heterocylic,alkyl, bicyclic heterocycle, aryl; R2 represents C1-3 alkyl, halogen or hydrogen; R3 represents a fluorinated straight or branched alkyl group of 1-6 carbon atoms and salts and solvates thereof, in particular, physiol. acceptable solvates and salts thereof. These compds. are agonists at the Adenosine A1 receptor. Thus, 5'-deoxy-5'-fluoro-N-(tetrahydro-pyran-4-yl)-adenosine was prepared and tested as adenosine A1 receptor (equipotent concentration ratio relative to NECA = 1.9).

IT **223774-67-2P 223774-68-3P 223774-69-4P**
223774-71-8P 223774-72-9P 223774-74-1P
223774-75-2P 223774-76-3P 223774-77-4P
223774-78-5P 223774-85-4P 223774-88-7P
223774-90-1P 223774-91-2P 223774-92-3P

223774-93-4P 224045-30-1P 224045-32-3P
(preparation of deoxyfluoro nucleosides as adenosine A1 receptors)

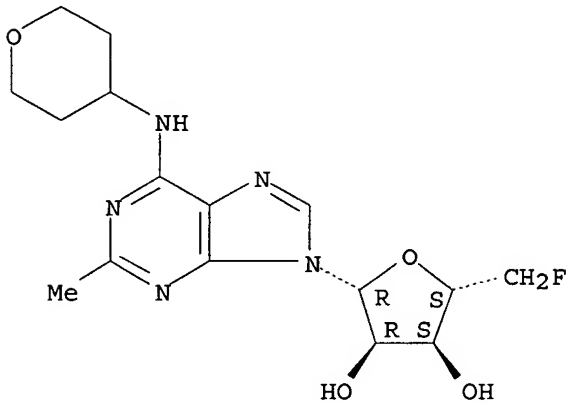
RN 223774-67-2 HCAPLUS
CN Adenosine, 5'-deoxy-5'-fluoro-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



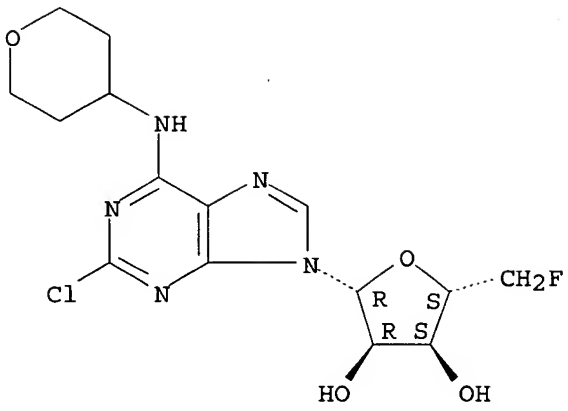
RN 223774-68-3 HCAPLUS
CN Adenosine, 5'-deoxy-5'-fluoro-2-methyl-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



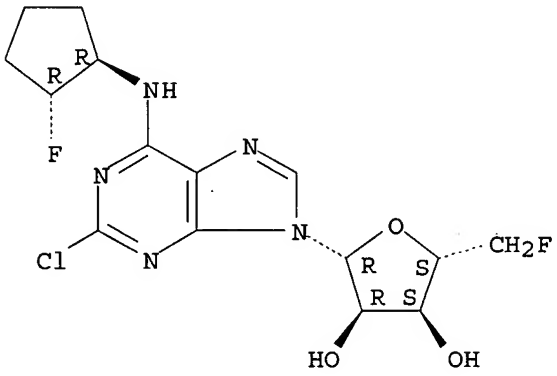
RN 223774-69-4 HCAPLUS
CN Adenosine, 2-chloro-5'-deoxy-5'-fluoro-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



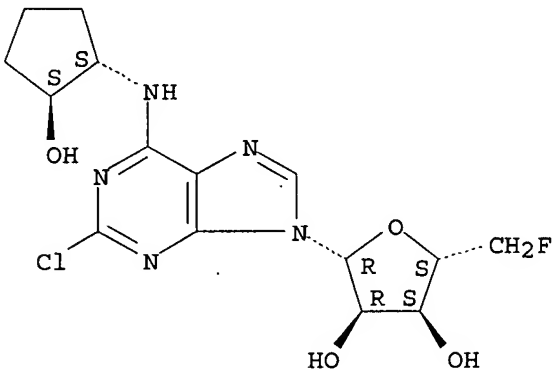
RN 223774-71-8 HCAPLUS
CN Adenosine, 2-chloro-5'-deoxy-5'-fluoro-N-[(1R,2R)-2-fluorocyclopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 223774-72-9 HCAPLUS
CN Adenosine, 2-chloro-5'-deoxy-5'-fluoro-N-[(1S,2S)-2-hydroxycyclopentyl]- (9CI) (CA INDEX NAME)

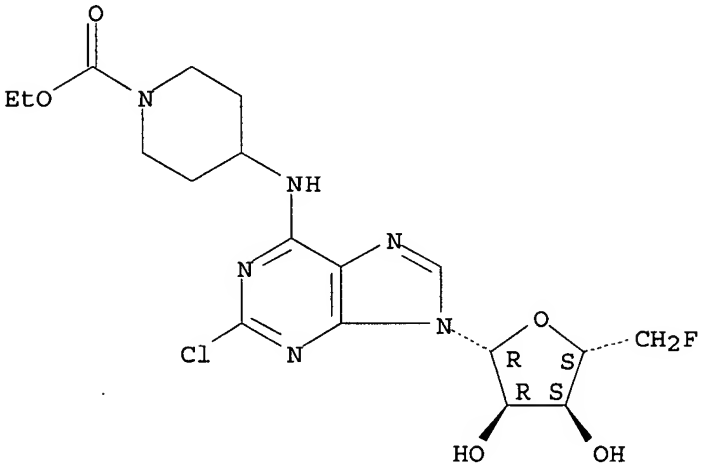
Absolute stereochemistry.



RN 223774-74-1 HCAPLUS

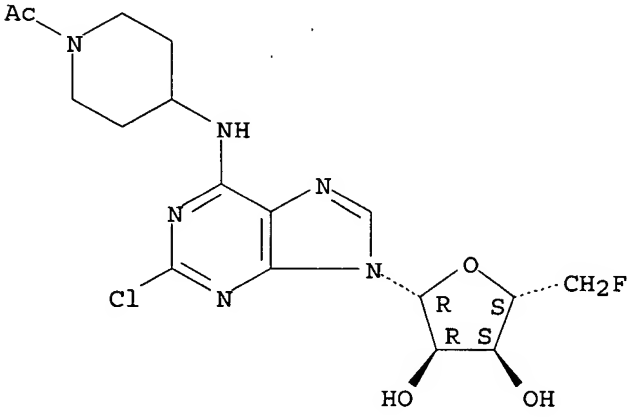
CN 1-Piperidinecarboxylic acid, 4-[[2-chloro-9-(5-deoxy-5-fluoro-β-D-ribofuranosyl)-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



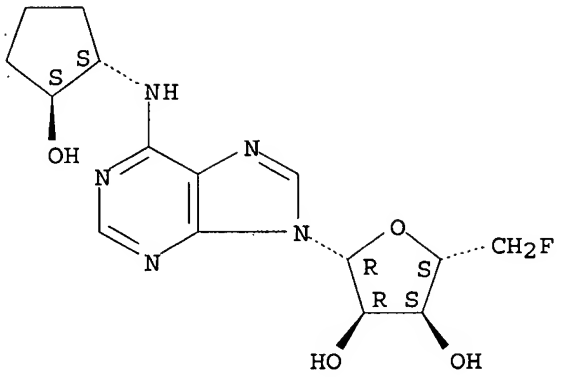
RN 223774-75-2 HCAPLUS
CN Adenosine, N-(1-acetyl-4-piperidinyl)-2-chloro-5'-deoxy-5'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



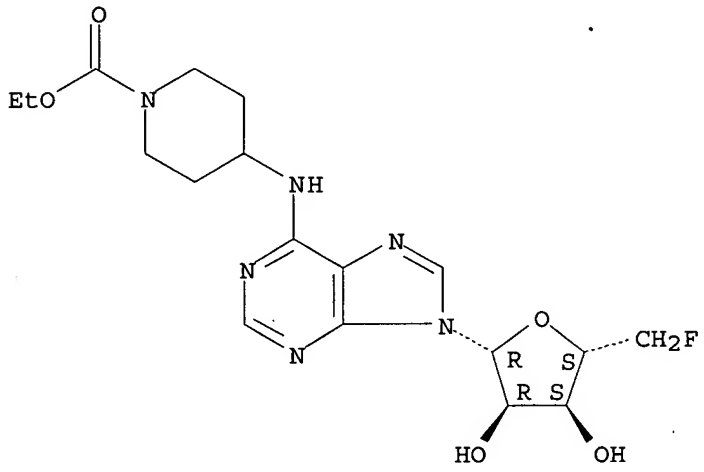
RN 223774-76-3 HCAPLUS
CN Adenosine, 5'-deoxy-5'-fluoro-N-[(1S,2S)-2-hydroxycyclopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



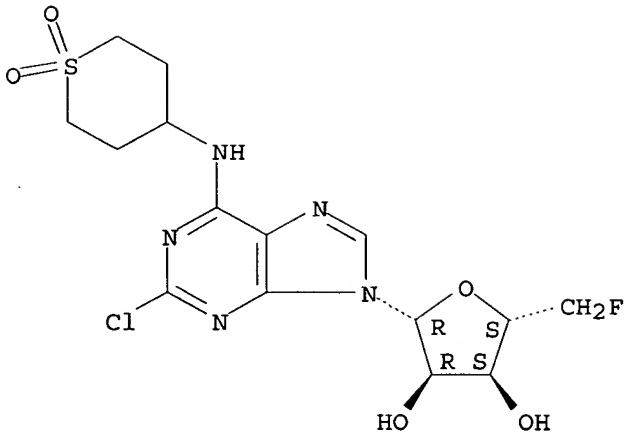
RN 223774-77-4 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-(5-deoxy-5-fluoro-β-D-ribofuranosyl)-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



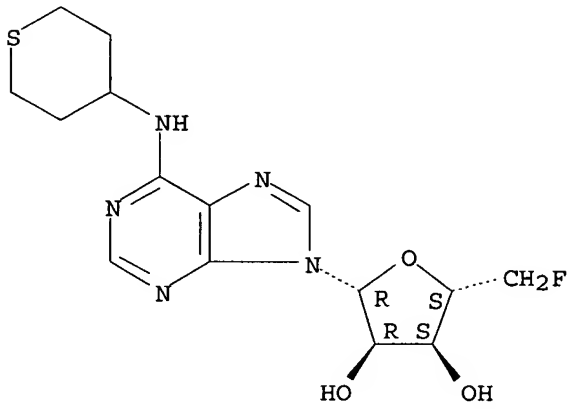
RN 223774-78-5 HCAPLUS
CN Adenosine, 2-chloro-5'-deoxy-5'-fluoro-N-(tetrahydro-1,1-dioxido-2H-thiopyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



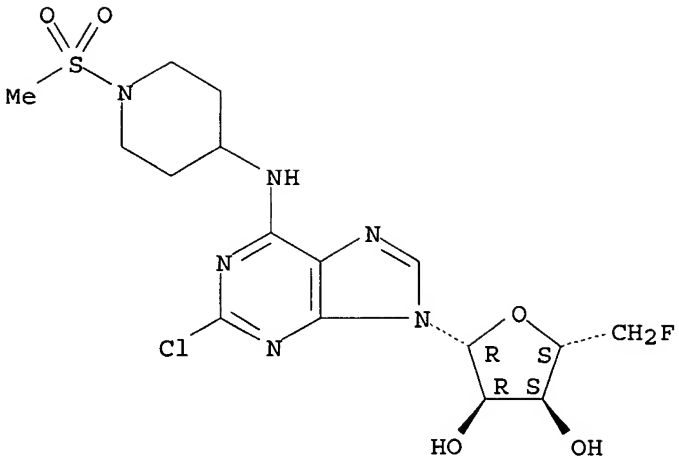
RN 223774-85-4 HCAPLUS
CN Adenosine, 5'-deoxy-5'-fluoro-N-(tetrahydro-2H-thiopyran-4-yl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



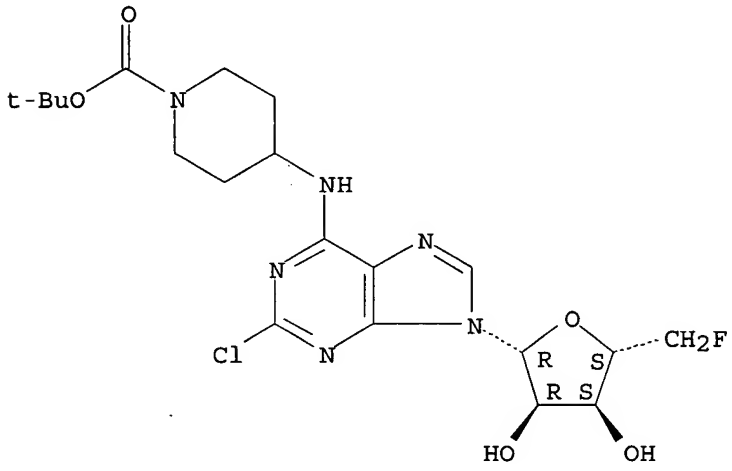
RN 223774-88-7 HCAPLUS
CN Adenosine, 2-chloro-5'-deoxy-5'-fluoro-N-[1-(methylsulfonyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



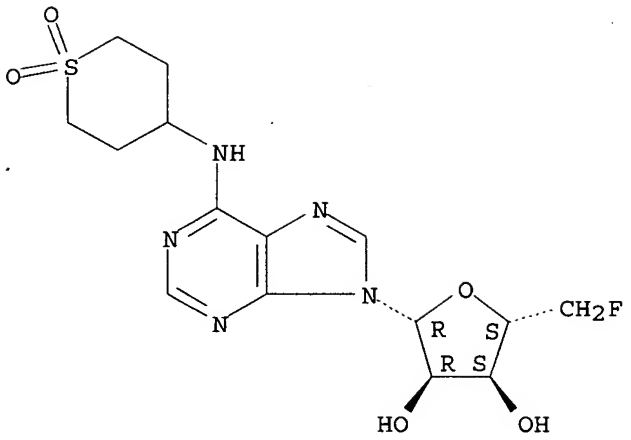
RN 223774-90-1 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[2-chloro-9-(5-deoxy-5-fluoro-β-D-ribofuranosyl)-9H-purin-6-yl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



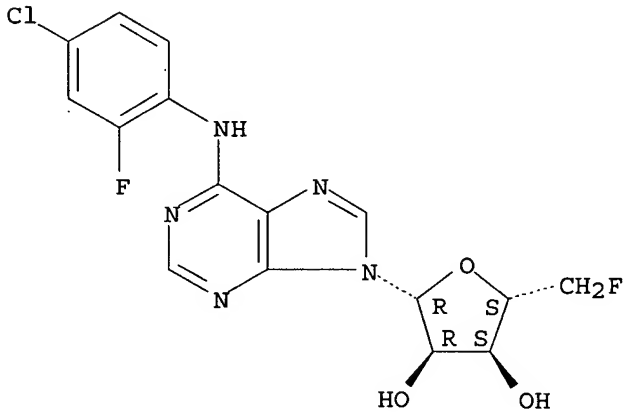
RN 223774-91-2 HCAPLUS
CN Adenosine, 5'-deoxy-5'-fluoro-N-(tetrahydro-1,1-dioxido-2H-thiopyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



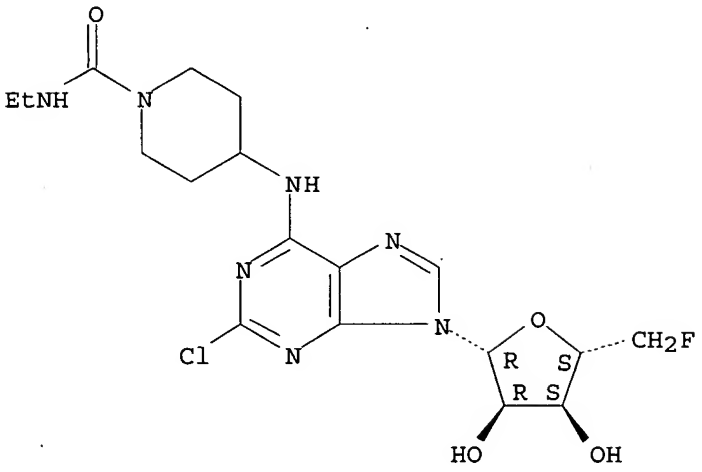
RN 223774-92-3 HCAPLUS
CN Adenosine, N-(4-chloro-2-fluorophenyl)-5'-deoxy-5'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



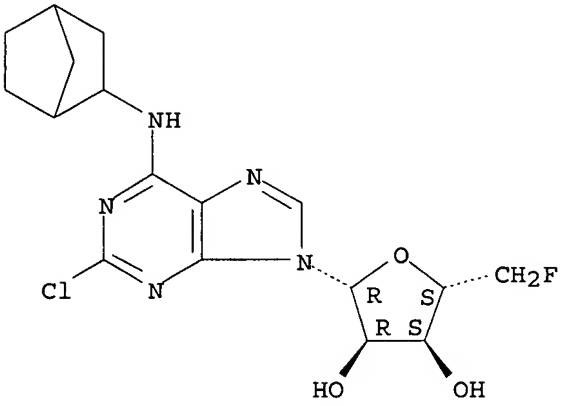
RN 223774-93-4 HCAPLUS
CN Adenosine, 2-chloro-5'-deoxy-N-[1-[(ethylamino)carbonyl]-4-piperidinyl]-5'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



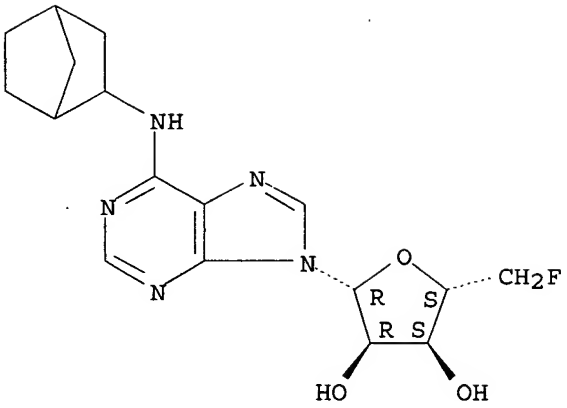
RN 224045-30-1 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-2-chloro-5'-deoxy-5'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



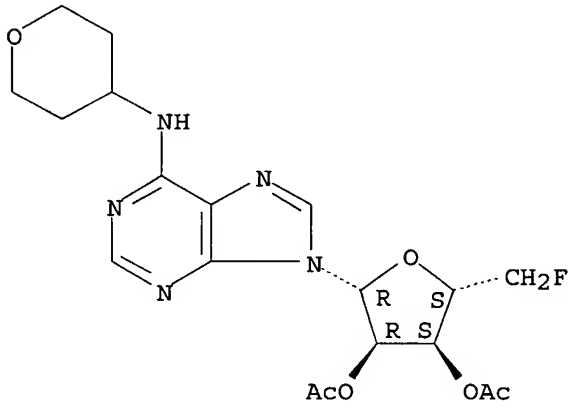
RN 224045-32-3 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-deoxy-5'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



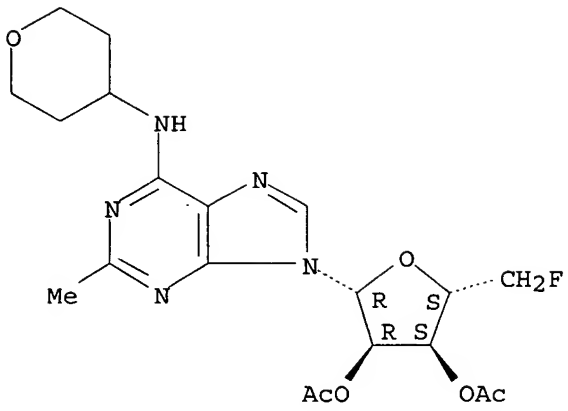
IT **223774-96-7P 223774-98-9P**
(preparation of deoxyfluoro nucleosides as adenosine A1 receptors)
RN 223774-96-7 HCAPLUS
CN Adenosine, 5'-deoxy-5'-fluoro-N-(tetrahydro-2H-pyran-4-yl)-, 2',3'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 223774-98-9 HCAPLUS
CN Adenosine, 5'-deoxy-5'-fluoro-2-methyl-N-(tetrahydro-2H-pyran-4-yl)-, 2',3'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-00
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT **223774-67-2P 223774-68-3P 223774-69-4P**
223774-70-7P **223774-71-8P 223774-72-9P**
223774-74-1P 223774-75-2P 223774-76-3P
223774-77-4P 223774-78-5P 223774-79-6P
223774-81-0P 223774-82-1P 223774-83-2P 223774-84-3P
223774-85-4P 223774-87-6P **223774-88-7P**
223774-89-8P **223774-90-1P 223774-91-2P**
223774-92-3P 223774-93-4P 224045-28-7P
224045-30-1P 224045-32-3P
(preparation of deoxyfluoro nucleosides as adenosine A1 receptors)
IT 1426-59-1P 151266-35-2P 169190-83-4P 223756-94-3P
223761-82-8P 223761-83-9P 223774-94-5P 223774-95-6P
223774-96-7P 223774-97-8P **223774-98-9P**
223774-99-0P 223775-01-7P 223775-03-9P 223775-04-0P
223775-05-1P 223775-07-3P 223775-08-4P
(preparation of deoxyfluoro nucleosides as adenosine A1 receptors)

L39 ANSWER 9 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:13 HCAPLUS
DOCUMENT NUMBER: 128:30047
TITLE: 5'-Substituted Adenosine Analogs as New High-Affinity Partial Agonists for the Adenosine A1 Receptor
AUTHOR(S): van der Wenden, Eleonora M.; Carnielli, Marta; Roelen, Harlof C. P. F.; Lorenzen, Anna; von Kuenzel, Jacobien K.; IJzerman, Adriaan P.
CORPORATE SOURCE: Div. Medicinal Chemistry, Leiden/Amsterdam Center for Drug Research, Leiden, 2300 RA, Neth.
SOURCE: Journal of Medicinal Chemistry (1998), 41(1), 102-108
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 5'-(Alkylthio)-, 5'-(methylseleno)-, and 5'-(alkylamino)-substituted analogs of N6-cyclopentyladenosine (CPA) were synthesized in 30-50% overall yields. The affinities of these compds. for the adenosine A1 and A2A receptors were determined in rat brain membranes. The 5'-substituted CPA analogs proved selective

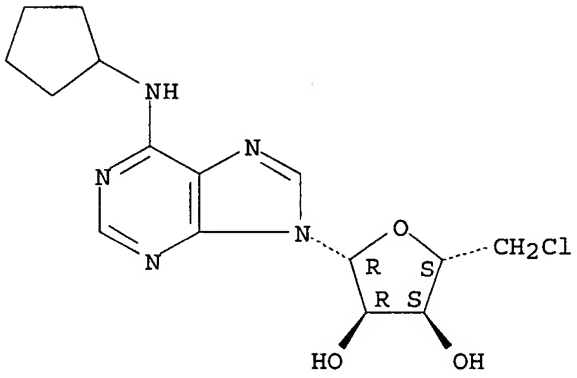
for the adenosine A1 receptors, displaying affinities in the nanomolar range. The compds. were also evaluated for their ability to stimulate [35S]GTPγS binding, also in rat brain membranes. The Ki values in receptor binding studies corresponded well to the EC50 values thus obtained. Intrinsic activities of the compds. were tested in vitro by determining the GTP shift in receptor binding studies as well as the maximal binding of [35S]GTPγS. It appeared that the 5'-thio and 5'-seleno derivs. in particular behaved as partial agonists.

IT **103626-57-9**
(substituted adenosine analogs as new high-affinity partial agonists for adenosine A1 receptor)

RN 103626-57-9 HCAPLUS

CN Adenosine, 5'-chloro-N-cyclopentyl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-3 (Pharmacology)
Section cross-reference(s): 33

IT 41552-82-3 **103626-57-9**
(substituted adenosine analogs as new high-affinity partial agonists for adenosine A1 receptor)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:623045 HCAPLUS
DOCUMENT NUMBER: 127:278413
TITLE: Preparation of nucleosides for treating disorders related to cytokines in mammals
INVENTOR(S): Knutsen, Lars; Olsen, Uffe Bang; Bowler, Andrew Neil
PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.
SOURCE: PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9733591 A1 19970918 WO 1997-DK108
1997
0312
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU,
CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,
MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,
TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU,
TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI,
FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

WO 9733590 A1 19970918 WO 1997-DK107
1997
0312
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU,
CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,
MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,
TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU,
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RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI,
FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9720224 A1 19971001 AU 1997-20224
1997
0312

AU 9720225 A1 19971001 AU 1997-20225
1997
0312

ZA 9702190 A 19971010 ZA 1997-2190
1997
0313

ZA 9702193 A 19971021 ZA 1997-2193
1997
0313

PRIORITY APPLN. INFO.: DK 1996-293 A
1996
0313

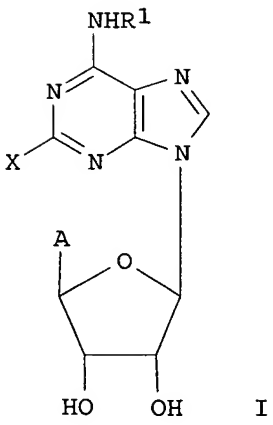
DK 1996-591 A
1996
0521

DK 1996-590
1996
0521

WO 1997-DK107 W
1997
0312

WO 1997-DK108 W
1997
0312

OTHER SOURCE(S): MARPAT 127:278413
GI



I

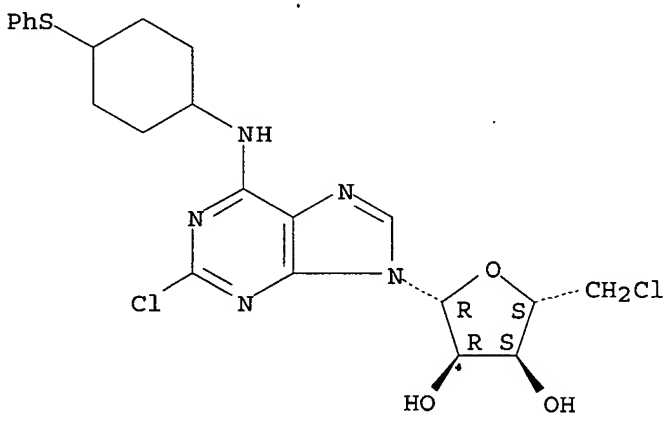
AB Preparation of nucleosides I (R1 = heterocycle, imino; X = H, halo, amino, perhalomethyl, cyano, alkyl, alkoxy, alkylthio, alkylamino, Ph; A = vinyl, CH2R2, R2 = Oh, H, Cl, Br, F, CN, NH2, MeO) for treating disorders related to cytokines such as TNFα in mammals. The disorder is an auto-immune disorder, inflammation, arthritis, multiple sclerosis, stroke, osteoporosis, septic shock or menstrual complications. Thus, 2-chloro-N-methoxyadenosine was prepared and tested for its auto-immune disorder and showed LPS-induced TNFα inhibition rat whole blood (IC50 = 3.0 μM).

IT **169190-76-5P**
(preparation of nucleosides for treating disorders related to cytokines in mammals)

RN 169190-76-5 HCAPLUS

CN Adenosine, 2,5'-dichloro-5'-deoxy-N-[4-(phenylthio)cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K031-70
ICS C07H019-167

CC 33-9 (Carbohydrates)

IT 13406-53-6P 32464-89-4P 151666-10-3P 154493-16-0P
154493-18-2P 154493-20-6P 154493-22-8P 154493-25-1P
154493-26-2P 169190-46-9P 169190-48-1P 169190-51-6P

169190-54-9P 169190-55-0P 169190-56-1P 169190-57-2P
169190-60-7P 169190-61-8P 169190-62-9P 169190-63-0P
169190-64-1P 169190-65-2P 169190-66-3P 169190-68-5P
169190-69-6P 169190-70-9P 169190-71-0P **169190-76-5P**
169190-80-1P 169190-82-3P 196496-76-1P 196496-78-3P
196496-80-7P 196496-82-9P 196496-83-0P 196496-84-1P
196496-86-3P 196496-91-0P 196496-93-2P 196496-97-6P
196496-98-7P 196497-01-5P 196497-10-6P 196497-15-1P
196497-19-5P 196497-24-2P 196497-28-6P
(preparation of nucleosides for treating disorders related to cytokines in mammals)

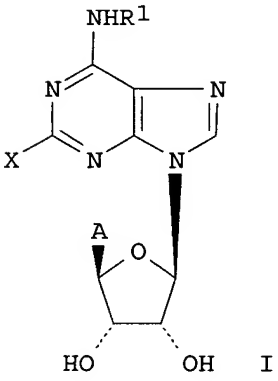
L39 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:867585 HCAPLUS
DOCUMENT NUMBER: 123:286531
TITLE: Preparation of adenosine derivatives for treatment of central nervous system diseases
INVENTOR(S): Lau, Jesper; Knutsen, Lars Jacob Stray
PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9507921	A1	19950323	WO 1994-DK344	19940915
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5589467	A	19961231	US 1994-306232	19940914
CA 2171940	AA	19950323	CA 1994-2171940	19940915
AU 9476519	A1	19950403	AU 1994-76519	19940915
AU 678053	B2	19970515		
EP 719275	A1	19960703	EP 1994-926815	19940915
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 11511436	T2	19991005	JP 1994-508922	19940915
ZA 9407201	A	19960318	ZA 1994-7201	19940916
FI 9601219	A	19960515	FI 1996-1219	1996

					0315
NO 9601071	A	19960515	NO 1996-1071		
					1996
					0315
PRIORITY APPLN. INFO.:			DK 1993-1043	A	
					1993
					0917
			DK 1994-310	A	
					1994
					0316
			WO 1994-DK344	W	
					1994
					0915

OTHER SOURCE(S): MARPAT 123:286531

GI



I

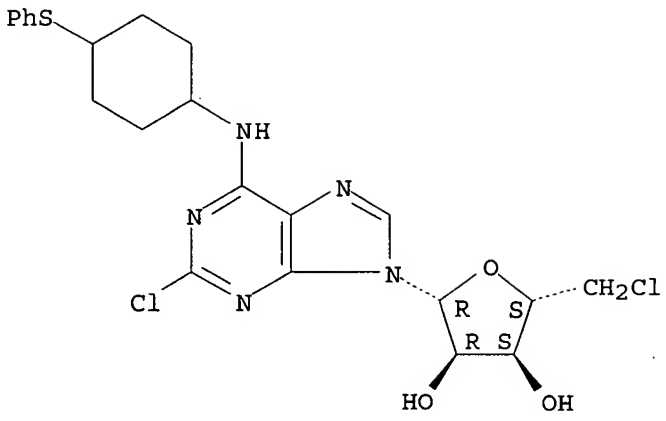
AB The title compds. I [X is halogen, amino, perhalomethyl, cyano, C1-6-alkoxy, C1-6-alkylthio or C1-6-alkylamino; A is Me, halomethyl, cyanomethyl, aminomethyl, vinyl, methylthiomethyl or methoxymethyl; R1 is selected from optionally substituted N-bonded heterocyclics] are prepared 2,5'-Dichloro-5'-deoxy-N-(1-piperidinyl)adenosine (II) (preparation given) showed ED50 of 0.4 mg/Kg against DMCM-induced seizures in in animals. In the in vitro test for the binding to the adenosine A1 receptors, II showed Ki value of 6.4 nM.

IT **169190-76-5P**
(preparation of adenosine derivs. for treatment of central nervous system diseases)

RN 169190-76-5 HCAPLUS

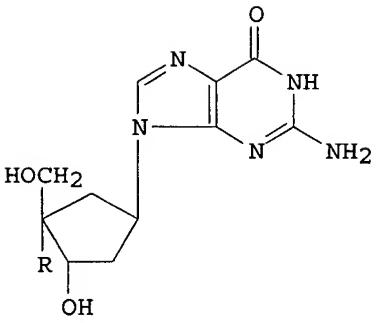
CN Adenosine, 2,5'-dichloro-5'-deoxy-N-[4-(phenylthio)cyclohexyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-16
ICS C07H019-167; A61K031-70
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 169190-46-9P 169190-47-0P 169190-48-1P 169190-49-2P
169190-50-5P 169190-51-6P 169190-52-7P 169190-53-8P
169190-54-9P 169190-55-0P 169190-56-1P 169190-57-2P
169190-58-3P 169190-59-4P 169190-60-7P 169190-61-8P
169190-62-9P 169190-63-0P 169190-64-1P 169190-65-2P
169190-66-3P 169190-67-4P 169190-68-5P 169190-69-6P
169190-70-9P 169190-71-0P 169190-72-1P 169190-73-2P
169190-74-3P 169190-75-4P **169190-76-5P**
(preparation of adenosine derivs. for treatment of central nervous system diseases)

L39 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:315219 HCAPLUS
DOCUMENT NUMBER: 120:315219
TITLE: Chiral carbocyclic nucleosides: the synthesis and antiviral activity of 4'-hydroxy and 4'-fluorocarbocyclic-2'-deoxyguanosines
AUTHOR(S): Borthwick, Alan D.; Biggadike, Keith; Paternoster, Ian L.; Coates, Jonathan A. V.; Knight, David J.
CORPORATE SOURCE: Dep. Med. Chem., Glaxo Group Res., Greenford/Middlesex, UB6 OHE, UK
SOURCE: Bioorganic & Medicinal Chemistry Letters (1993), 3(12), 2577-80
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I, R=OH
II, R=F

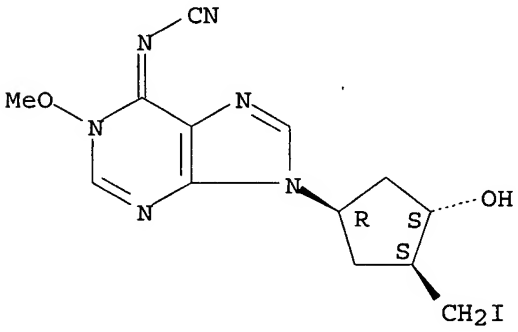
AB The chiral carbocyclic nucleosides I and II were prepared from aristeromycin. The 4'α-hydroxy compound I displays good antiviral activity against HSV-1 and HSV-2 with low toxicity.

IT **127454-22-2P**
(preparation and conversion to 4',5'-olefin)

RN 127454-22-2 HCAPLUS

CN Cyanamide, [1,9-dihydro-9-[3-hydroxy-4-(iodomethyl)cyclopentyl]-1-methoxy-6H-purin-6-ylidene]-, [1R-(1α,3β,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



CC 1-5 (Pharmacology)
Section cross-reference(s): 33

IT **127454-22-2P**
(preparation and conversion to 4',5'-olefin)

L39 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1993:473005 HCAPLUS
DOCUMENT NUMBER:	119:73005
TITLE:	C-2 functionalized N6-cyclosubstituted adenosines: highly selective agonists for the adenosine A1 receptor
AUTHOR(S):	Nair, Vasu; Fasbender, Allen J.
CORPORATE SOURCE:	Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE:	Tetrahedron (1993), 49(11), 2169-84 CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE:	Journal
LANGUAGE:	English

OTHER SOURCE(S): CASREACT 119:73005
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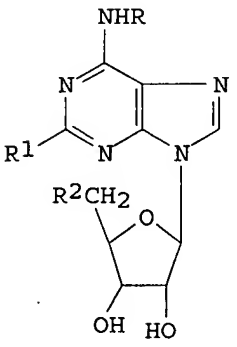


I

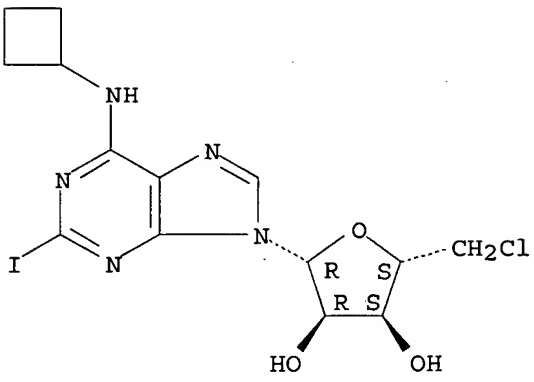
AB Synthesis of novel N6-cyclosubstituted isoguanosines, e.g. I (R = cyclopentyl, R1 = iodo, OH, R2 = OH; R = cyclopentyl, R1 = iodo, R2 = Cl; R = 3-noradamantyl, R1 = H, Cl, R2 = OH; R = pyrrolidino, R1 = H, R2 = OH; R = cyclobutyl, cyclohexyl, cycloheptyl, endo-2-norbornyl, R1 = R2 = OH), and related C(2) functionalized compds. utilizing methodols. with key thermal radical and photochem. steps developed in our laboratory is described. Data on the affinities of these new compds. for the adenosine A1 and A2 receptors clearly show that a number of N6-cyclosubstituted isoguanosines show excellent A1 agonist activity with the best activity and selectivity being associated with five-membered ring mono- or bicyclic systems at the N6-position. Interestingly, 2-iodo-N6-cyclopentyladenosine also shows excellent A1 receptor binding and A2/A1 selectivity.

IT **149007-81-8P 149007-82-9P**
(preparation and affinity of, for adenosine receptors)

RN 149007-81-8 HCAPLUS

CN Adenosine, 5'-chloro-N-cyclobutyl-5'-deoxy-2-iodo- (9CI) (CA INDEX NAME)

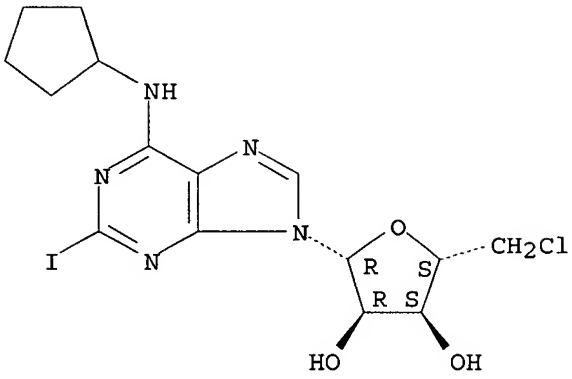
Absolute stereochemistry.



RN 149007-82-9 HCAPLUS

CN Adenosine, 5'-chloro-N-cyclopentyl-5'-deoxy-2-iodo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

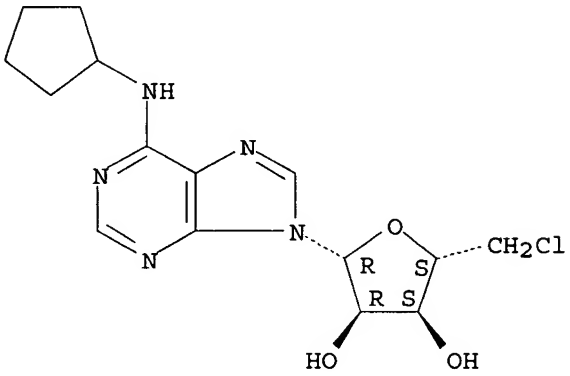


CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 36799-21-0P 133501-99-2P 133502-00-8P 133502-22-4P
133502-23-5P 133502-24-6P 133502-25-7P 133502-26-8P
149007-77-2P 149007-79-4P 149007-80-7P **149007-81-8P**
149007-82-9P 149007-83-0P 149007-85-2P 149007-86-3P
(preparation and affinity of, for adenosine receptors)

L39 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:207931 HCAPLUS
DOCUMENT NUMBER: 116:207931
TITLE: Agonist activity of 2- and 5'-substituted adenosine analogs and their N6-cycloalkyl derivatives at A1- and A2-adenosine receptors coupled to adenylate cyclase
AUTHOR(S): Daly, John W.; Padgett, William L.
CORPORATE SOURCE: Lab. Bioorg. Chem., Natl. Inst. Diabetes Dig. Kidney Dis., Bethesda, MD, 20892, USA
SOURCE: Biochemical Pharmacology (1992), 43(5), 1089-93
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The activity of N6-cycloalkyl derivs. of adenosine, 2-chloroadenosine, 5'-chloroadenosine, and N-ethylcarboximidoadenosine (NECA) and of 2-fluoroadenosine and 5-methylthioadenosines were compared at the A1-adenosine receptor inhibitory to adenylate cyclase in rat fat cell membranes and at the A2A-adenosine receptors stimulatory to adenylate cyclase in rat PC12 cell membranes. The N6-cycloalkyl derivs. in all cases were more potent (4-23-fold) than the parent compound at the A1 receptor, and were less potent (1.6-11-fold) than the parent compound at the A2A receptor. N6-Cyclopentyl-5'-chloroadenosine was the most selective agonist (900-fold) for the A1 receptor, whereas 2-fluoroadenosine was the only agonist with some selectivity (4.8-fold) for the A2A receptor. 5'-Methylthioadenosine was a weak agonist at both adenosine receptors. A 2-fluoro derivative of 5'-methylthioadenosine was somewhat more potent. Affinities of these analogs for inhibition of binding of radioligands to rat brain A1 and A2A receptors are presented.
IT **103626-57-9**
(purinoceptor agonist activity of, mol. structure in relation to)

RN 103626-57-9 HCAPLUS
CN Adenosine, 5'-chloro-N-cyclopentyl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2-2 (Mammalian Hormones)
IT 146-77-0, 2-Chloroadenosine 146-78-1 892-48-8 2457-80-9, 5'-Methylthioadenosine 35920-39-9, NECA 37739-05-2 41552-82-3, N6-Cyclopentyladenosine 103201-24-7
103626-57-9 110022-90-7
(purinoceptor agonist activity of, mol. structure in relation to)

L39 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:143930 HCAPLUS
DOCUMENT NUMBER: 114:143930
TITLE: Preparation of 5'N, 6-disubstituted adenosines from inosines
INVENTOR(S): Bridges, Alexander J.
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: U.S., 7 pp. Cont. of U.S. Ser. No. 34,125, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4962194	A	19901009	US 1988-260202	19881019
PRIORITY APPLN. INFO.:			US 1987-34125 B1	19870402

OTHER SOURCE(S): CASREACT 114:143930; MARPAT 114:143930
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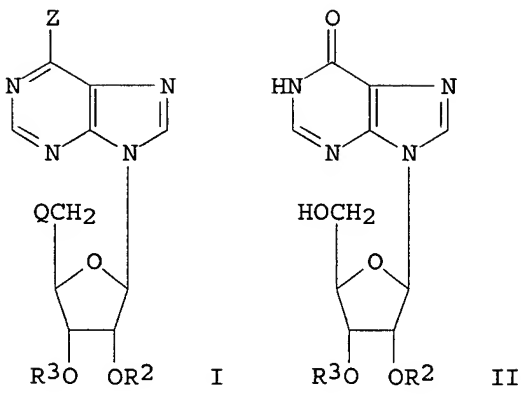


I II

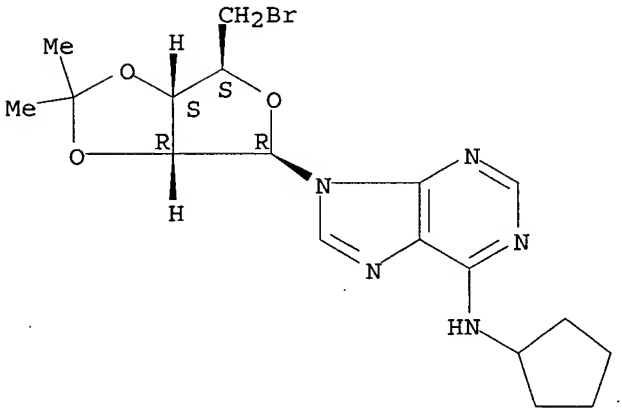
AB The title compds. [I; R2, R3 = H, alkyl, alkanoyl, Bz; or R2R3 = alkylidene; Z = RS(O)q, (un)substituted NH2; R = alkyl, (hetero)aryl, aralkyl; q = 0, 2; Q = H, halo, cyano, N3, NH2, alkoxy, acyloxy, thioalkyl, H2NNH, HONH, phosphino, dialkyl or diarylcuprato] are prepared by (1) bromination of inosine derivs. (II; R2, R3 = as defined above, excluding R2 = R3 = H) with Ar3PBr2 or (ArO)3PBr2 (Ar = aryl) followed by reaction with RSH (R = as defined above) to give I (Z = RS, Q = Br), (2) oxidation of the latter to I [Z = RS(O)q Q = Br], (3) amination of the latter with amines to give I [Z = (un)substituted NH2, Q = Br], and (4) treatment of the latter with a nucleophile. Some I are useful as neuroleptics, analgesics, cardiotonics, antihypertensives, antilipolytics, antihyperlipemics, antiinflammatory agents, antithrombotic or antiembolic agents (no data). Thus, bromination of 2',3'-isopropylideneinosine with Br/Ph3P in pyridine followed by reaction with PhSH gave I (Z = PhS, Q = Br, R1R3 = CMe2) which was oxidized with m-ClC6H4C(O)OOH in CHCl3 in the presence of NaHCO3 to I (Z = PhSO2; R, R2, R3 = as defined above). Amination of the latter with cyclopentylamine in the presence of Et3N in CHCl3 and thiolation of the product I (Z = cyclopentylamino; Q, R2, R3 = as defined above) with NaSMe in Me2SO followed by hydrolysis gave I (Z = cyclopentylamino, Q = MeS, R2 = R3 = H).

IT **117325-48-1P**
(preparation and thiolation of, by sodium thiomethoxide)

RN 117325-48-1 HCAPLUS

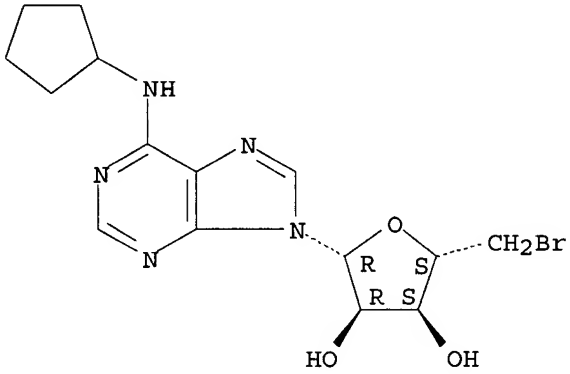
CN Adenosine, 5'-bromo-N-cyclopentyl-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **117325-49-2P**
(preparation of, as pharmaceutical)
RN 117325-49-2 HCAPLUS
CN Adenosine, 5'-bromo-N-cyclopentyl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-167
ICS C07H019-20
INCL 536026000
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT **117325-48-1P**
(preparation and thiolation of, by sodium thiomethoxide)
IT 103626-35-3P 103626-43-3P **117325-49-2P**
(preparation of, as pharmaceutical)

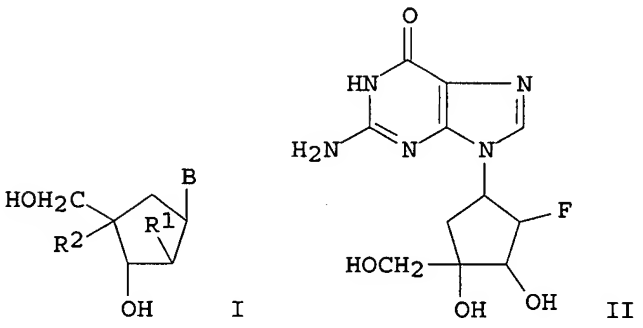
L39 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:571783 HCAPLUS
DOCUMENT NUMBER: 113:171783
TITLE: Preparation and formulation of cyclopentane derivatives and carbocyclic analogs of nucleosides as virucides
INVENTOR(S): Borthwick, Alan David; Biggakike, Keith
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 345076	A1	19891206	EP 1989-305577	19890602
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 8935936	A1	19891207	AU 1989-35936	19890601
AU 618813	B2	19920109		
DK 8902692	A	19891204	DK 1989-2692	19890602
FI 8902719	A	19891204	FI 1989-2719	19890602
NO 8902252	A	19891204	NO 1989-2252	19890602
NO 169652	B	19920413		
NO 169652	C	19920722		
JP 02085284	A2	19900326	JP 1989-139374	19890602
ZA 8904192	A	19900829	ZA 1989-4192	19890602

PRIORITY APPLN. INFO.: GB 1988-13148 A 19880603

OTHER SOURCE(S): MARPAT 113:171783
GI



AB Title compds. I (R1 = H, F, HO; R2 = F, HO, C1-6 alkoxy; B = purine base), salts and solvates thereof, useful as virucides (no data), were prepared (±)-(1α,2α,3β,4β)-I

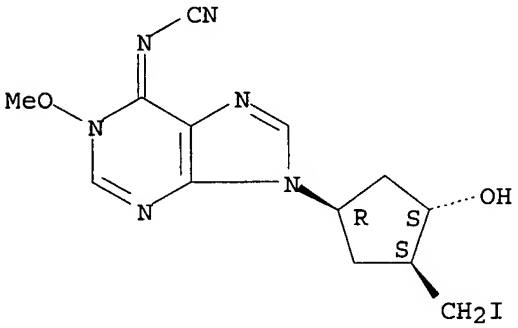
(R1 = F; R2 = HO; B = 2-amino-6-methoxy-9H-purin-9-yl) (preparation given) was heated at 85° in 2N HCl to give (±)-(1'α,2'α,3'β,4'β)-II. Pharmaceutical compns. comprising I are given.

IT **127454-22-2P**
(preparation of, as intermediate for carbocyclic nucleoside analog virucides)

RN 127454-22-2 HCAPLUS

CN Cyanamide, [1,9-dihydro-9-[3-hydroxy-4-(iodomethyl)cyclopentyl]-1-methoxy-6H-purin-6-ylidene]-, [1R-(1α,3β,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IC ICM C07D473-16
ICS C07D473-18; C07D473-32; C07D473-34; A61K031-52

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 63

IT 127454-10-8P 127454-11-9P 127454-12-0P 127454-13-1P
127454-14-2P 127454-15-3P 127454-16-4P 127454-17-5P
127454-18-6P 127454-19-7P 127454-20-0P 127454-21-1P
127454-22-2P 127454-23-3P 127454-24-4P 127454-25-5P
127454-26-6P 127454-27-7P 127454-28-8P 127454-29-9P
127454-30-2P 127475-50-7P 127475-51-8P 127475-52-9P
127514-35-6P 127514-36-7P 127849-00-7P 127870-82-0P
(preparation of, as intermediate for carbocyclic nucleoside analog virucides)

L39 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:115221 HCAPLUS

DOCUMENT NUMBER: 112:115221

TITLE: 2-Chloro-N6-[3H]cyclopentyladenosine ([3H]CPPA) - a high affinity agonist radioligand for A1 adenosine receptors

AUTHOR(S): Klotz, Karl Norbert; Lohse, Martin J.; Schwabe, Ulrich; Cristalli, Gloria; Vittori, Sauro; Grifantini, Mario

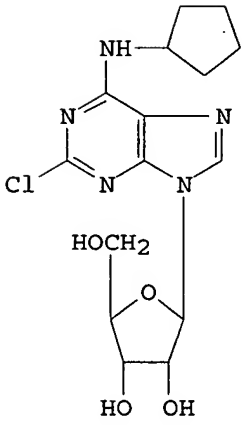
CORPORATE SOURCE: Pharmakol. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.

SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1989), 340(6), 679-83
CODEN: NSAPCC; ISSN: 0028-1298

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

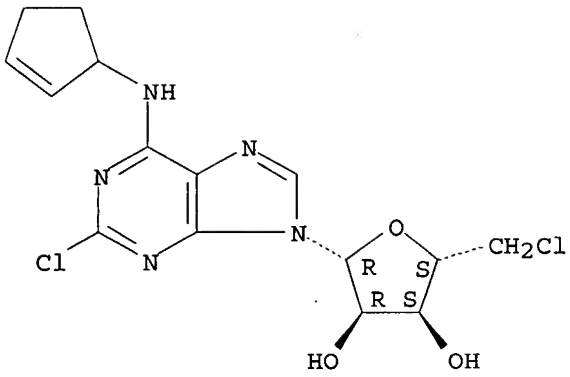
AB The tritiated analog of 2-chloro-N6-cyclopentyladenosine (CCPA) (I), an adenosine derivative with subnanomolar affinity and a 10,000-fold selectivity for A1 adenosine receptors, has been examined as a new agonist radioligand. [3H]CCPA was prepared with a specific radioactivity of 1.58 TBq/mmol (43 Ci/mmol) and bound in a reversible manner to A1 receptors from rat brain membranes with a high affinity KD value of 0.2 nmol/L. In the presence of GTP, a KDvalue of 13 nmol/L was determined for the low affinity state for agonist binding. Competition of several adenosine receptor agonists and antagonists for [3H]CCPA binding to rat brain membranes confirmed binding to an A1 receptor. Solubilized A1 receptors bound [3H]CCPA with similar affinity for the high affinity state. At solubilized receptors a reduced association rate was observed in the presence of MgCl2, as has been shown for the agonist [3H]N6-phenylisopropyladenosine ([3H]PIA). [3H]CCPA was also used for detection of A1 receptors in rat cardiomyocyte membranes, a tissue with a very low receptor d. Kd-Value of 0.4 nmol-L and a Bmax-value of 16 fmol-platelet membranes, no specific binding of [3H]CCPA was measured at concns. up to 400 nmol/L, indicating that A2 receptors did not bind [3H]CCPA. Based on the subnanomolar affinity and the high selectivity for A1 receptors, [3H]CCPA proved to be a useful agonist radioligand for characterization of A1 adenosine receptors also in tissues with very low receptor d.

IT **125730-29-2P**
(preparation and reduction with tritium of)

RN 125730-29-2 HCAPLUS

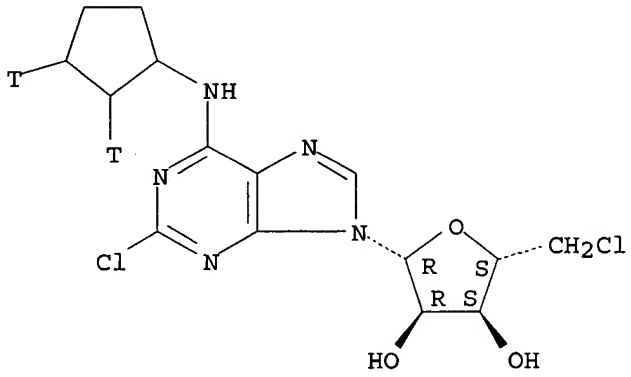
CN Adenosine, 2,5'-dichloro-N-2-cyclopenten-1-yl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



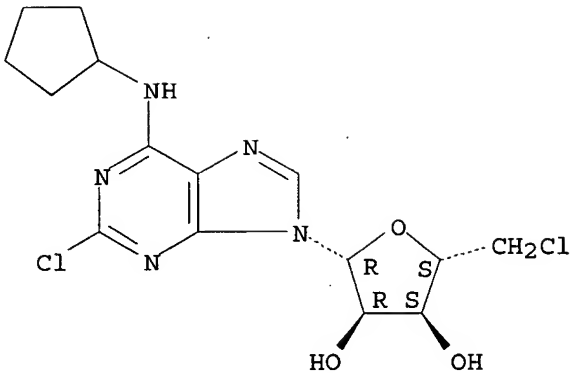
IT **125730-26-9P**
(preparation of and purinergic A1 receptors labeling by)
RN 125730-26-9 HCAPLUS
CN Adenosine, 2,5'-dichloro-N-(cyclopentyl-2,3-t2)-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



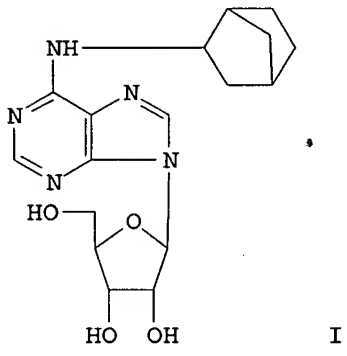
IT **125730-27-0**
(purinergic A1 receptors labeling by)
RN 125730-27-0 HCAPLUS
CN Adenosine, 2,5'-dichloro-N-cyclopentyl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 9-8 (Biochemical Methods)
Section cross-reference(s): 2, 28
IT 125730-28-1P **125730-29-2P**
(preparation and reduction with tritium of)
IT 125730-25-8P **125730-26-9P**
(preparation of and purinergic A1 receptors labeling by)
IT 37739-05-2 **125730-27-0**
(purinergic A1 receptors labeling by)

L39 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:33329 HCAPLUS
DOCUMENT NUMBER: 110:33329
TITLE: N6-Bicycloalkyladenosines with unusually high potency and selectivity for the adenosine A1 receptor
AUTHOR(S): Trivedi, B. K.; Bridges, A. J.; Patt, W. C.; Priebe, S. R.; Bruns, R. F.
CORPORATE SOURCE: Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (1989), 32(1), 8-11
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The influence of stereochem. on the affinity of a series of adenosines substituted with a 2-norbornyl group at N6 towards

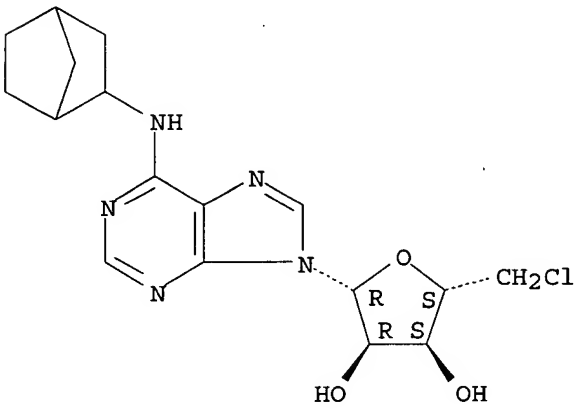
adenosine A1 and A2 receptors was examined These compds. can be considered to be conformationally locked derivs. of N6-cyclopentyl- or N6-cyclohexyladenosine. N6-(2-endo-Norbornyl)adenosine had higher affinity and selectivity for the A1 receptor than N6-(2-exo-norbornyl)adenosine. The 1R,2S,4S isomer of N6-(2-endo-norbornyl)adenosine (I) had still higher affinity and selectivity, which could be further increased by 5'-chloro-5'-deoxy substitution. The latter compound showed the greatest A1 affinity (Ki 0.24 nM) and highest A1 selectivity (16,000-fold) yet reported for an adenosine agonist. In addition, [3H]N6-[(1R,2S,4S)-2-norbornyl]adenosine was found to bind to rat brain A1 receptors with a Kd of 0.33 nM, suggesting potential utility as an improved A1 agonist radioligand. The geometrical requirements for A1 receptor affinity in this series were used to refine a model of the N6-domain of the A1 receptor.

IT **103626-26-2 103626-57-9 117773-75-8**
117773-76-9
(adenosine A1-receptor binding affinity of, selectivity in)

RN 103626-26-2 HCAPLUS

CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-chloro-5'-deoxy- (9CI) (CA INDEX NAME)

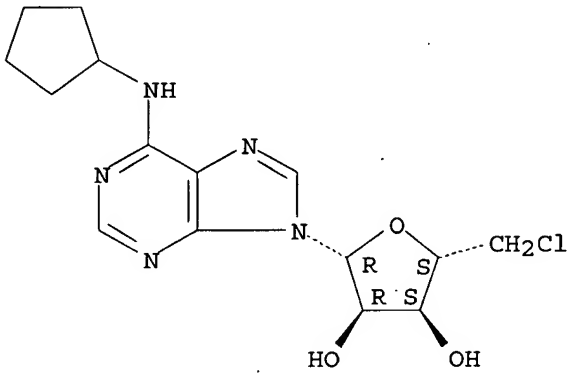
Absolute stereochemistry.



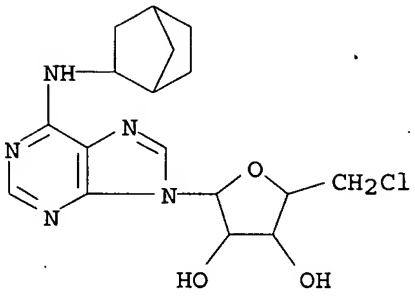
RN 103626-57-9 HCAPLUS

CN Adenosine, 5'-chloro-N-cyclopentyl-5'-deoxy- (9CI) (CA INDEX NAME)

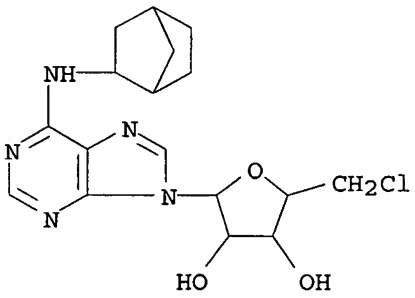
Absolute stereochemistry.



RN 117773-75-8 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-chloro-5'-deoxy-, (1S-endo)- (9CI) (CA INDEX NAME)

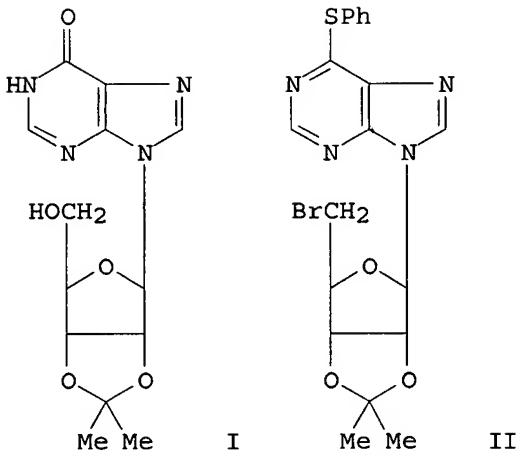


RN 117773-76-9 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-chloro-5'-deoxy-, (1R-endo)- (9CI) (CA INDEX NAME)



CC 1-3 (Pharmacology)
Section cross-reference(s): 2
IT 41552-82-3 **103626-26-2 103626-57-9**
117773-72-5 117773-73-6 117773-74-7 **117773-75-8**
117773-76-9
(adenosine A1-receptor binding affinity of, selectivity in)

L39 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:611373 HCAPLUS
DOCUMENT NUMBER: 109:211373
TITLE: Triarylphosphine-phosphite dibromide. A convenient reagent for the preparation of S-arylthioinosines and N6,5'-disubstituted adenosine derivatives from inosine
AUTHOR(S): Bridges, Alexander J.
CORPORATE SOURCE: Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 43805, USA
SOURCE: Nucleosides & Nucleotides (1988), 7(3), 375-83
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:211373
GI



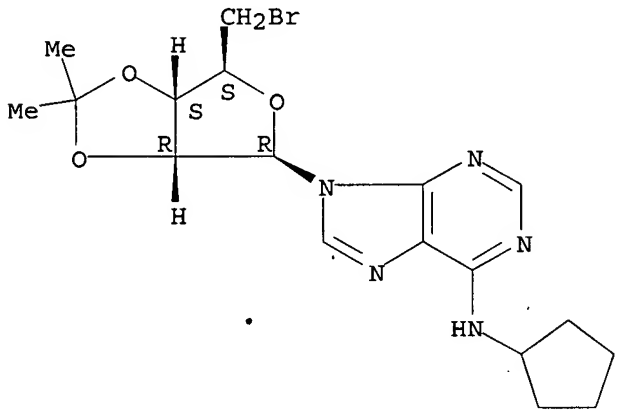
AB Isopropylideneinosine I reacts with Ph3PBr2 or (PhO)3PBr2 and PhSH to give 5'-bromo-S-phenylthioinosine (II) which is a versatile precursor for 5',N6-disubstituted adenosine derivs.

IT **117325-48-1P**
(preparation and reactions of)

RN 117325-48-1 HCAPLUS

CN Adenosine, 5'-bromo-N-cyclopentyl-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

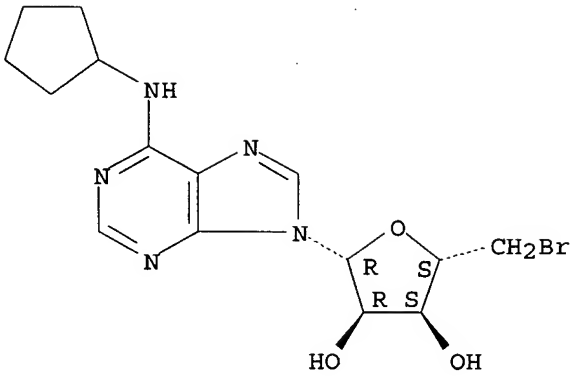


IT **117325-49-2P**
(preparation of)

RN 117325-49-2 HCAPLUS

CN Adenosine, 5'-bromo-N-cyclopentyl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



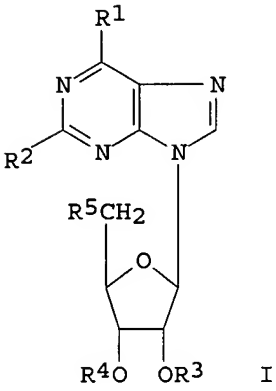
CC 33-9 (Carbohydrates)
IT 117325-47-0P **117325-48-1P**
(preparation and reactions of)
IT 103626-35-3P 103626-43-3P 117325-44-7P 117325-45-8P
117325-49-2P 117325-50-5P 117325-51-6P 117325-52-7P
(preparation of)

L39 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:67628 HCAPLUS
DOCUMENT NUMBER: 106:67628
TITLE: N6-(bicycloalkyl)adenosines
INVENTOR(S): Trivedi, Bharat
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 181128	A2	19860514	EP 1985-307715	1985 1025
EP 181128	A3	19870520		
EP 181128	B1	19891004		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4714697	A	19871222	US 1985-772983	1985 0909
CA 1254888	A1	19890530	CA 1985-492865	1985 1011
AU 8548775	A1	19860501	AU 1985-48775	1985 1016
AU 576717	B2	19880901		
ZA 8508000	A	19860528	ZA 1985-8000	1985 1017
DK 8504883	A	19860427	DK 1985-4883	1985

				1024
DK 159854	B	19901217		
DK 159854	C	19910513		
ES 548237	A1	19860516	ES 1985-548237	
				1985
				1025
JP 61143395	A2	19860701	JP 1985-237760	
				1985
				1025
AT 46911	E	19891015	AT 1985-307715	
				1985
				1025
PRIORITY APPLN. INFO.:			US 1984-665216	A
				1984
				1026
			US 1985-772983	A
				1985
				0909
			EP 1985-307715	A
				1985
				1025

OTHER SOURCE(S): MARPAT 106:67628
GI



I

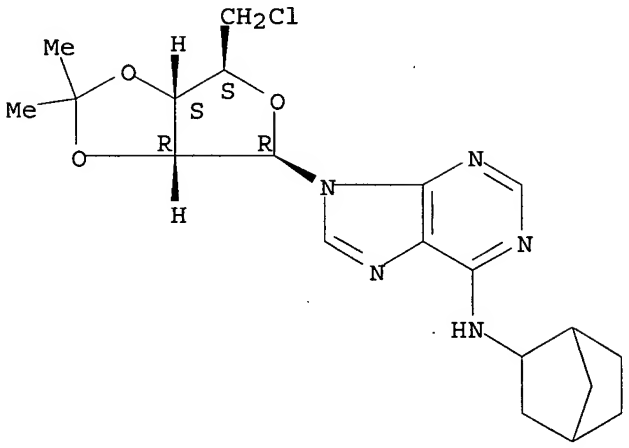
AB Adenosines I (R1 = bicycloalkenylamino, bicycloalkylamino; R2 = H, halo, SH, alkylthio, etc.; R3 and R4 are H, alkanoyl, PhCO, substituted benzoyl, or R3R4 = alkylidene; R5 = halo, H, OH, acyloxy, etc.) were prepared, and they exhibited analgesic and antiinflammatory activity. 6-Chloropurine was treated with 2-aminonorbornane, and the adenine deriv obtained was glycosylated to give I (R1 = 2-norbornylamino, R2 = R3 = R4 = R5 = H).

IT **103626-25-1P**
(preparation and reaction of)

RN 103626-25-1 HCAPLUS

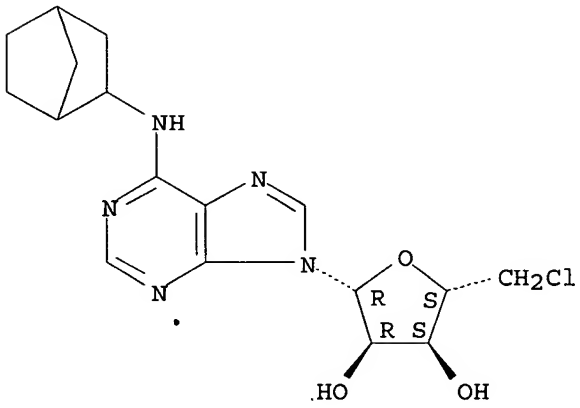
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-chloro-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **103626-26-2P**
(preparation of, as analgesic and antiinflammatory agent)
RN 103626-26-2 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-chloro-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-167
ICS A61K031-70
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 103626-24-0P **103626-25-1P** 103626-28-4P
(preparation and reaction of)
IT 97826-51-2P **103626-26-2P** 103626-27-3P 103626-29-5P
(preparation of, as analgesic and antiinflammatory agent)

L39 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:479310 HCAPLUS
DOCUMENT NUMBER: 105:79310
TITLE: N6-Substituted deoxyribose analogs of adenosines
INVENTOR(S): Hamilton, Harriet W.; Bristol, James A.; Moos, Walter; Trivedi, Bharat K.; Taylor, Michael;

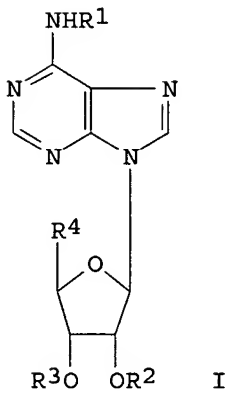
Patt, William C.
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: Eur. Pat. Appl., 69 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 181129	A2	19860514	EP 1985-307717	1985 1025
EP 181129	A3	19870513		
EP 181129	B1	19890308		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AU 8548888	A1	19860508	AU 1985-48888	1985 1021
AU 575438	B2	19880728		
FI 8504153	A	19860427	FI 1985-4153	1985 1023
FI 81587	B	19900731		
FI 81587	C	19901112		
ZA 8508154	A	19860625	ZA 1985-8154	1985 1023
DK 8504884	A	19860427	DK 1985-4884	1985 1024
NO 8504278	A	19860428	NO 1985-4278	1985 1025
NO 165495	B	19901112		
NO 165495	C	19910220		
JP 61148194	A2	19860705	JP 1985-237759	1985 1025
ES 548238	A1	19861201	ES 1985-548238	1985 1025
AT 41158	E	19890315	AT 1985-307717	1985 1025
CA 1260931	A1	19890926	CA 1985-493849	1985 1025
CN 85108658	A	19860716	CN 1985-108658	1985 1026
CN 1013448	B	19910807		
ES 555142	A1	19871101	ES 1986-555142	1986 0520

PRIORITY APPLN. INFO.: US 1984-665217 A 1984 1026

US 1984-665232	A	1984 1026
US 1984-665233	A	1984 1026
US 1985-772315	A	1985 0906
EP 1985-307717	A	1985 1025

OTHER SOURCE(S): MARPAT 105:79310
GI



I

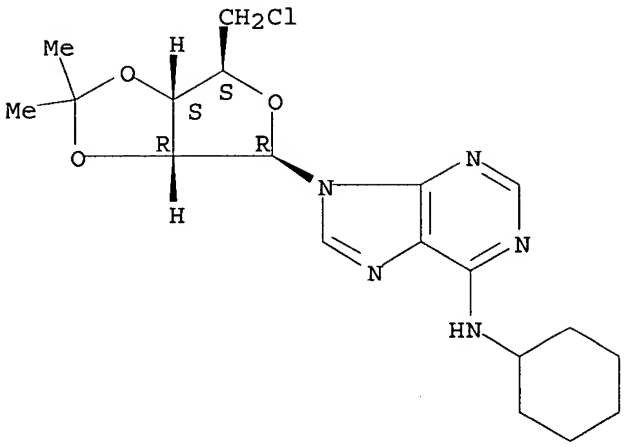
AB 5'-Deoxyadenosines I (R1 = cycloalkyl, CH2CHPh2, 1-indanyl, 1-tetralinyl, CHMeCH2Ph, 1-naphthylmethyl; R2 and R3 are H, alkyl, alkanoyl, etc.; R4 = Me, halomethyl, CH2SMe) were prepared, and they showed antipsychotic, antihypertensive, and analgesic activity. 6-(2,2-Diphenylethylamino)purine was treated with a 5-deoxyribose derivative to give I (R1 = CH2CHPh2, R2 = R3 = H, R4 = Me).

IT **103626-41-1P 103626-44-4P 103626-49-9P 103626-51-3P 103667-48-7P**
(preparation and reaction of)

RN 103626-41-1 HCAPLUS

CN Adenosine, 5'-chloro-N-cyclohexyl-5'-deoxy-2',3'-O-(1-methylethylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

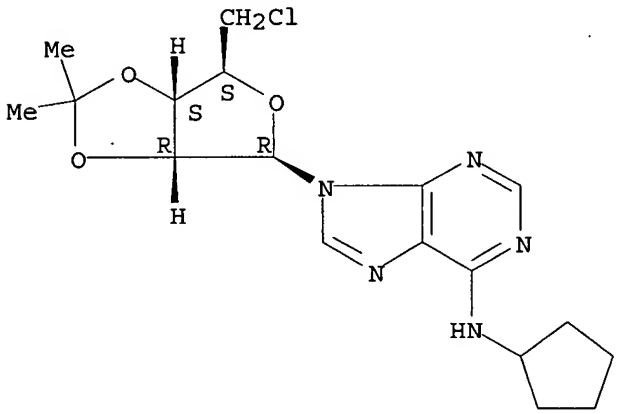
Absolute stereochemistry.



● HCl

RN 103626-44-4 HCAPLUS
CN Adenosine, 5'-chloro-N-cyclopentyl-5'-deoxy-2',3'-O-(1-methylethylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

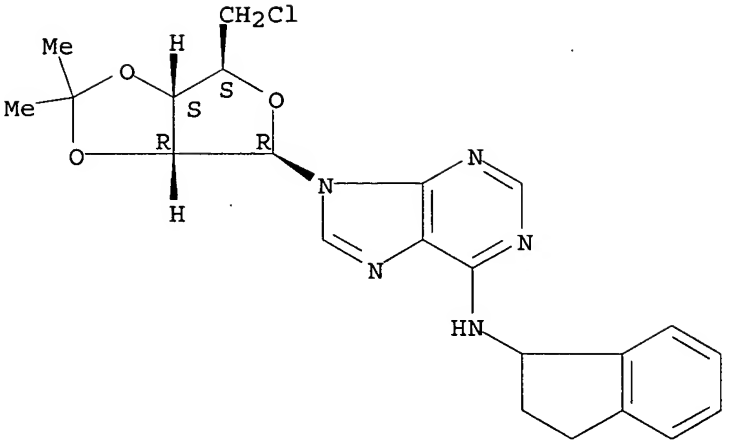
Absolute stereochemistry.



● HCl

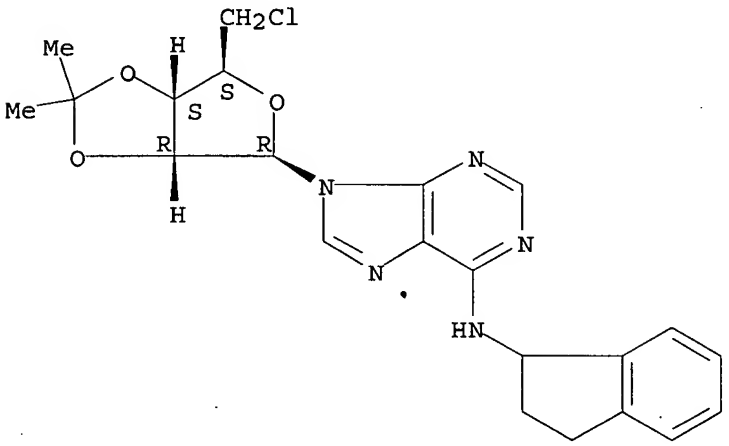
RN 103626-49-9 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 103626-51-3 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

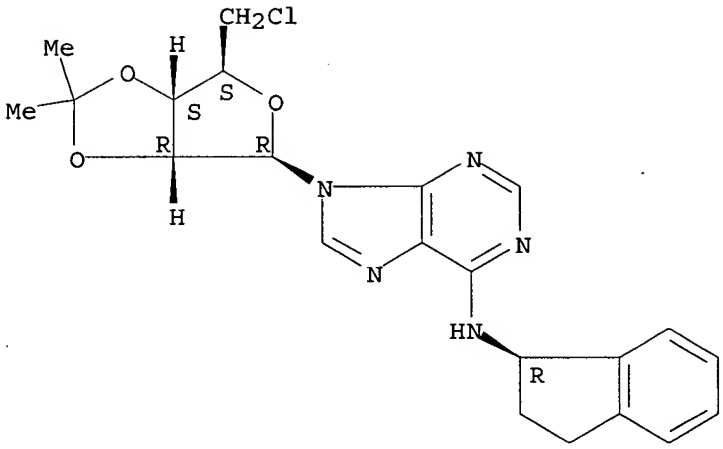
Absolute stereochemistry.



● HCl

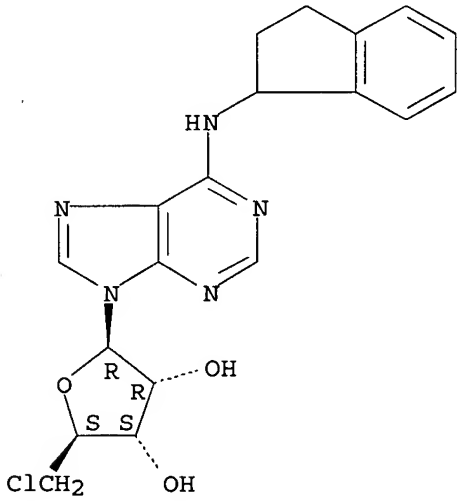
RN 103667-48-7 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



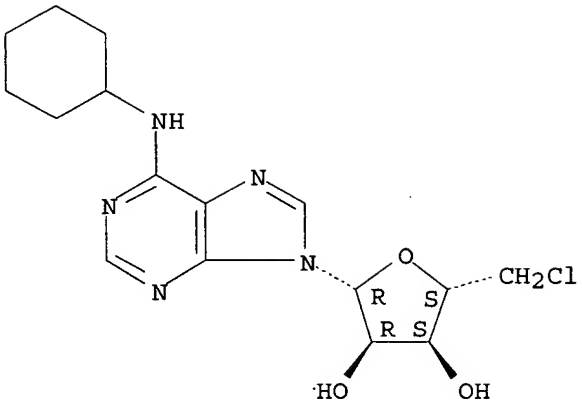
IT **103626-54-6P 103626-56-8P 103626-57-9P**
(preparation of, as a drug)
RN 103626-54-6 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



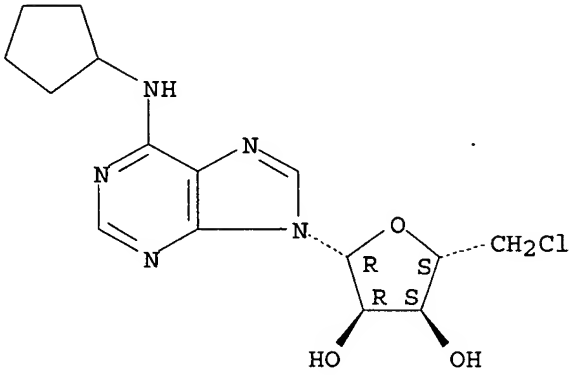
RN 103626-56-8 HCAPLUS
CN Adenosine, 5'-chloro-N-cyclohexyl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



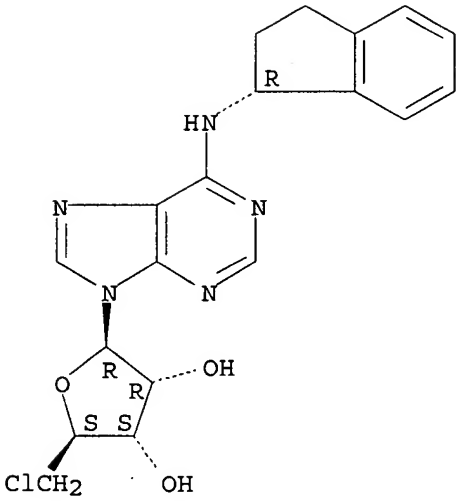
RN 103626-57-9 HCAPLUS
CN Adenosine, 5'-chloro-N-cyclopentyl-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **103667-47-6P**
(preparation of, as drug)
RN 103667-47-6 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)-, (R)- (9CI) (CA INDEX NAME)

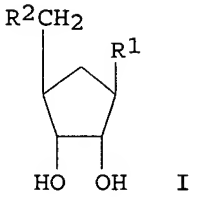
Absolute stereochemistry.



IC ICM C07H019-167
ICS A61K031-70
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 3369-66-2P 7674-45-5P 30154-66-6P 30302-57-9P 96323-21-6P
98383-40-5P 103626-31-9P 103626-33-1P 103626-36-4P
103626-39-7P **103626-41-1P** 103626-42-2P
103626-44-4P 103626-45-5P 103626-46-6P
103626-49-9P 103626-50-2P **103626-51-3P**
103626-53-5P 103626-58-0P 103626-60-4P 103626-62-6P
103626-63-7P 103626-64-8P 103639-11-8P 103654-17-7P
103667-48-7P 103729-37-9P
(preparation and reaction of)
IT 99798-09-1P 99798-10-4P 99798-11-5P 103626-30-8P
103626-32-0P 103626-34-2P 103626-35-3P 103626-37-5P
103626-38-6P 103626-40-0P 103626-43-3P 103626-47-7P
103626-48-8P 103626-52-4P **103626-54-6P** 103626-55-7P
103626-56-8P **103626-57-9P** 103626-59-1P
103626-61-5P
(preparation of, as a drug)
IT **103667-47-6P**
(preparation of, as drug)

L39 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:127766 HCAPLUS
DOCUMENT NUMBER: 102:127766
TITLE: Potential inhibitors of S-adenosylmethionine-dependent methyltransferases. 10. Base- and amino acid modified analogs of S-aristeromycinyl-L-homocysteine
AUTHOR(S): Houston, D. Michael; Matuszewska, Bozena; Borchardt, Ronald T.
CORPORATE SOURCE: Dep. Biochem., Univ. Kansas, Lawrence, KS, 66044, USA
SOURCE: Journal of Medicinal Chemistry (1985), 28(4), 478-82
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

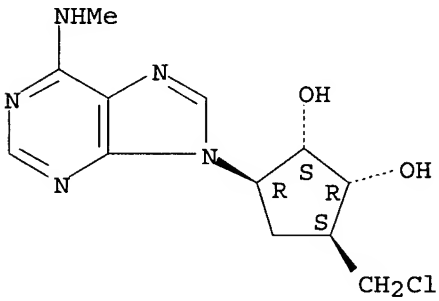
AB The title compds., I (R1 = adenine, 3-deazaadenine, 8-azaadenine, or N6-methyladenine; R2 = Cl or SCH2CH2CH(NH2)CO2H) were prepared and evaluated as inhibitors of catechol O-methyltransferase (II), phenylethanolamine N-methyltransferase (III), and histamine O-methyltransferase (IV). S-Deazaasteromycinyl-DL-homocysteine (I; R1 = 3-deazaadenine, R2 = D-SCH2CH2CH(NH2)CO2H) was a good inhibitor of III, whereas S-aristeromycinyl-D-homocysteine (I; R1 = adenine, R2 = D-SCH2CH2CH(NH2)CO2H) was a good inhibitor of IV. Apparently, structural requirements for binding S-aristeromycinyl-L-homocysteine are similar to those for binding S-adenosyl-L-homocysteine.

IT **94800-45-0P**
(preparation and reaction with homocysteinethiolactone)

RN 94800-45-0 HCAPLUS

CN 1,2-Cyclopentanediol, 3-(chloromethyl)-5-[6-(methylamino)-9H-purin-9-yl]-, [1S-(1α,2α,3β,5β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
Section cross-reference(s): 33

IT **94800-45-0P** 94842-38-3P
(preparation and reaction with homocysteinethiolactone)

=> d l40 1-23 ibib abs hitstr hitind

L40 ANSWER 1 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:165887 HCAPLUS
DOCUMENT NUMBER: 144:412818
TITLE: Antitrypanosomal Activity of

5'-Deoxy-5'-(iodo-methylene)adenosine and Related 6-N-Cyclopropyl-adenosine Analogs

AUTHOR(S): Rapp, Magdalena; Haubrich, Trisha A.; Perrault, Jacques; Mackey, Zachary B.; McKerrow, James H.; Chiang, Peter K.; Wnuk, Stanislaw F.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Florida International University, Miami, FL, 33199, USA

SOURCE: Journal of Medicinal Chemistry (2006), 49(6), 2096-2102
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:412818

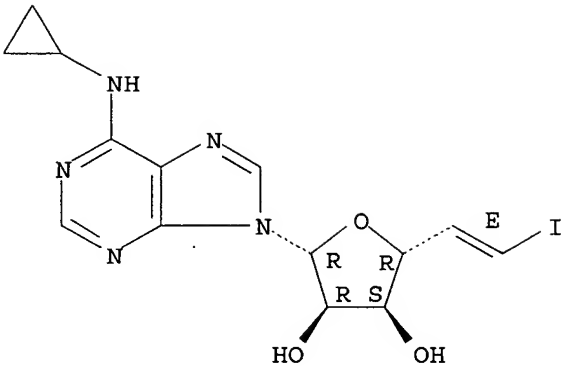
AB Treatment of the 6-N-cyclopropyl-2',3'-di-O-isopropylidene-adenosine 5'-aldehyde with sulfone-stabilized phosphonate or fluoro-phosphonate reagents followed by stannyl de-sulfonylation and subsequent iodo- or de-stannylation gave 6-N-cyclopropyl-5'-deoxy-5'-(iodo-methylene)adenosine (I) or its 5'-fluoromethylene analog. Treatment of the 5'-aldehyde with hydroxylamine or dibromo-methylene- or cyano-methylene-stabilized Wittig reagents and deprotection gave the oxime, 5'-cyano-methylene, and 5'-dibromo-methylene analogs. Dehydrobromination of 5'-dibromo-methylene analog gave acetylenic compound From the tested 6-N-cyclopropyl-adenosine analogs modified at the 5' carbon, the 5'-iodo-methylene I had the most potent activity against Trypanosoma brucei in vitro with an IC50 of 12 μg/mL. The IC50 value was 19 μg/mL for both the 5'-fluoromethylene and the 5'-cyano-methylene compds. The (E)-5'-deoxy-5'-(iodo-methylene)adenosine, a known inhibitor of AdoHcy hydrolase not modified with a cyclopropyl ring at 6-amino group, also inhibited Trypanosoma brucei with an IC50 of 9 μg/mL. In contrast to some other adenosine analogs modified at C5', the 6-N-cyclopropyl-adenosine analogs described here do not exhibit an inhibitory effect on AdoHcy hydrolase and displayed only marginal antiviral activity.

IT **883743-38-2P 883743-39-3P 883743-42-8P**
(preparation and antitrypanosomal activity of 5'-deoxy-5'-(iodo-methylene)adenosine and related cyclopropyl-adenosine analogs via Wittig and dehydrobromination reactions)

RN 883743-38-2 HCAPLUS

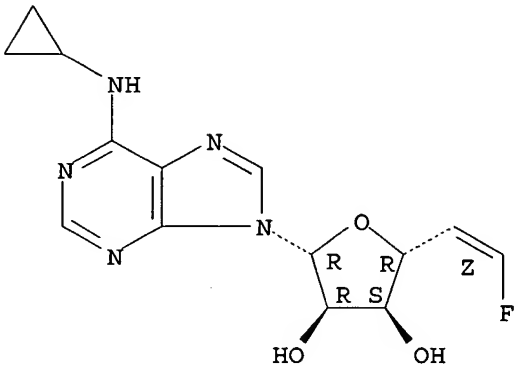
CN 9H-Purin-6-amine, N-cyclopropyl-9-[(5E)-5,6-dideoxy-6-iodo-β-D-ribo-hex-5-enofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



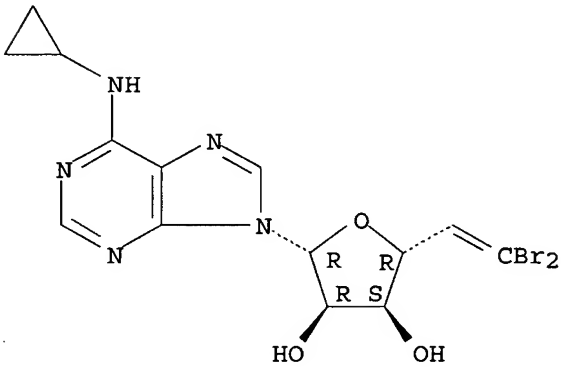
RN 883743-39-3 HCAPLUS
CN 9H-Purin-6-amine, N-cyclopropyl-9-[(5Z)-5,6-dideoxy-6-fluoro-β-D-ribo-hex-5-enofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 883743-42-8 HCAPLUS
CN 9H-Purin-6-amine, N-cyclopropyl-9-[6,6-dibromo-5,6-dideoxy-β-D-ribo-hex-5-enofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

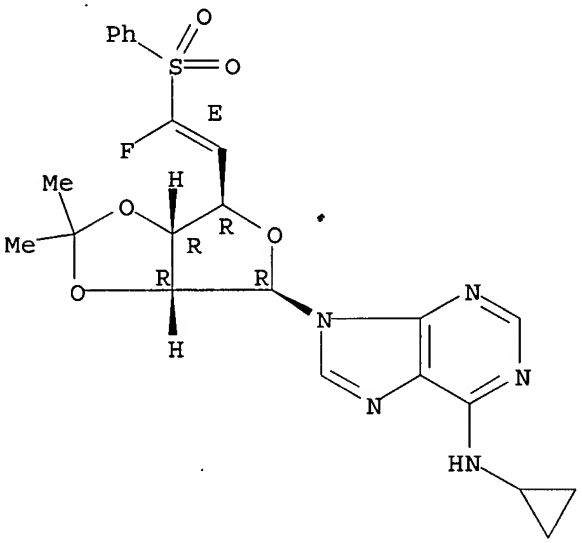


IT **883743-34-8P 883743-36-0P 883743-37-1P**

883743-41-7P
(preparation and antitrypanosomal activity of 5'-deoxy-5'-(iodomethylene)adenosine and related cyclopropyl-adenosine analogs via Wittig and dehydrobromination reactions)

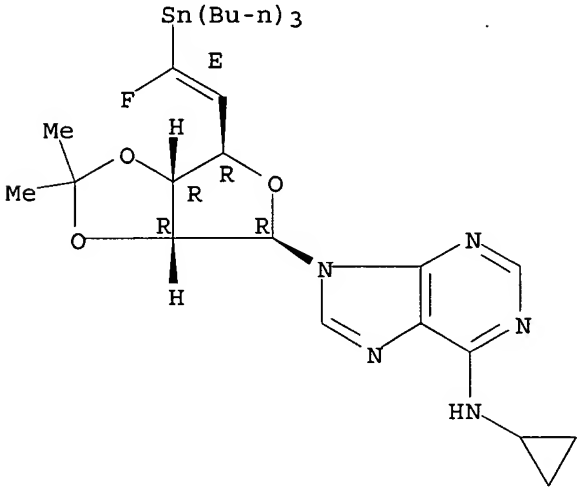
RN 883743-34-8 HCAPLUS
CN 9H-Purin-6-amine, N-cyclopropyl-9-[(5E)-5,6-dideoxy-6-fluoro-2,3-O-(1-methylethylidene)-6-(phenylsulfonyl)-β-D-ribo-hex-5-enofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



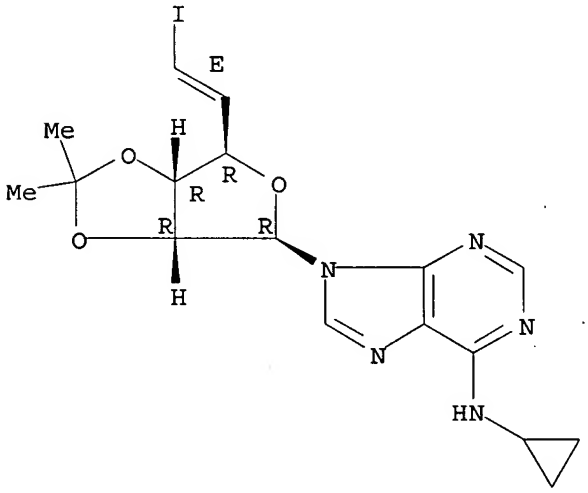
RN 883743-36-0 HCAPLUS
CN 9H-Purin-6-amine, N-cyclopropyl-9-[(5E)-5,6-dideoxy-6-fluoro-2,3-O-(1-methylethylidene)-6-(tributylstannyl)-β-D-ribo-hex-5-enofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



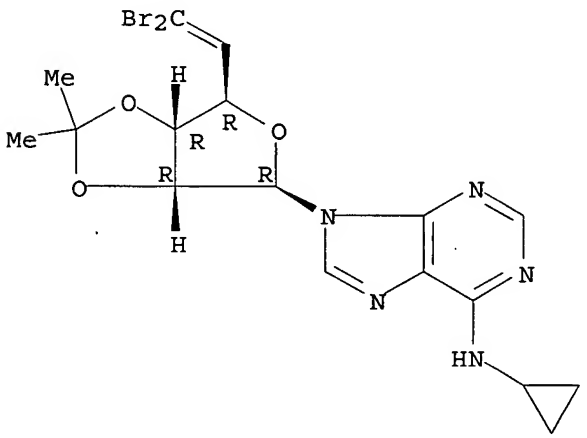
RN 883743-37-1 HCAPLUS
CN 9H-Purin-6-amine, N-cyclopropyl-9-[(5E)-5,6-dideoxy-6-iodo-2,3-O-(1-methylethylidene)-β-L-ribo-hex-5-enofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 883743-41-7 HCAPLUS
CN 9H-Purin-6-amine, N-cyclopropyl-9-[6,6-dibromo-5,6-dideoxy-2,3-O-(1-methylethylidene)-β-D-ribo-hex-5-enofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

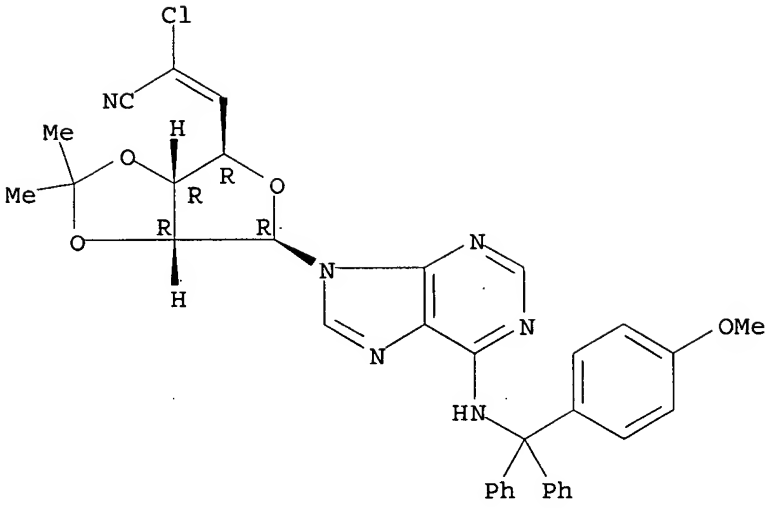


CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 7
IT 458566-36-4P 883743-29-1P 883743-32-6P **883743-38-2P**
883743-39-3P 883743-42-8P
(preparation and antitrypanosomal activity of 5'-deoxy-5'-(iodomethylene)adenosine and related cyclopropyl-adenosine analogs via Wittig and dehydrobromination reactions)
IT 97374-48-6P 883743-28-0P 883743-30-4P 883743-31-5P
883743-33-7P **883743-34-8P** 883743-35-9P

883743-36-0P 883743-37-1P 883743-41-7P
883743-43-9P
(preparation and antitrypanosomal activity of 5'-deoxy-5'-(iodomethylene)adenosine and related cyclopropyl-adenosine analogs via Wittig and dehydrobromination reactions)
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 2 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:87613 HCAPLUS
DOCUMENT NUMBER: 144:312280
TITLE: Inactivation of S-Adenosyl-L-homocysteine Hydrolase by 6'-Cyano-5',6'-didehydro-6'-deoxyhomoadenosine and 6'-Chloro-6'-cyano-5',6'-didehydro-6'-deoxyhomoadenosine. Antiviral and Cytotoxic Effects
AUTHOR(S): Guillerm, Georges; Muzard, Murielle; Glapski, Cedric; Pilard, Serge; De Clercq, Erik
CORPORATE SOURCE: Laboratoire de Chimie bioorganique, UMR 6519, UFR Sciences, Reims, 51687, Fr.
SOURCE: Journal of Medicinal Chemistry (2006), 49(4), 1223-1226
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:312280
AB 6'-Cyano-5',6'-didehydro-6'-deoxyhomoadenosine (E)-1, (Z)-1, and 6'-chloro-6'-cyano-5',6'-didehydro-6'-deoxyhomoadenosine (E)-2 were synthesized and tested as new mechanism-based inhibitors of AdoHcy hydrolase. Nucleoside (E)-1 was identified as a type I inhibitor of the enzyme, whereas inactivation of the enzyme by nucleosides (Z)-1 and (E)-2 was accompanied by the formation of a covalent labeling of AdoHcy hydrolase.
IT **880098-35-1P**
(preparation and antiviral and cytotoxic effects of 6'-cyano-5',6'-didehydro-6'-deoxyhomoadenosine and 6'-chloro-6'-cyano-5',6'-didehydro-6'-deoxyhomoadenosine as S-adenosyl-L-homocysteine hydrolase inhibitors)
RN 880098-35-1 HCAPLUS
CN β-D-ribo-Hept-5-enofuranurononitrile, 6-chloro-1,5,6-trideoxy-1-[6-[[(4-methoxyphenyl)diphenylmethyl]amino]-9H-purin-9-yl]-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 7
IT 128060-64-0P 880098-34-0P **880098-35-1P** 880098-36-2P
880098-37-3P
(preparation and antiviral and cytotoxic effects of
6'-cyano-5',6'-didehydro-6'-deoxyhomoadenosine and
6'-chloro-6'-cyano-5',6'-didehydro-6'-deoxyhomoadenosine as
S-adenosyl-L-homocysteine hydrolase inhibitors)
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 3 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:162706 HCAPLUS
DOCUMENT NUMBER: 140:199640
TITLE: Preparation of adenosine derivatives as partial and full agonists of A1 adenosine receptors
INVENTOR(S): Zablocki, Jeff; Palle, Venkata; Elzein, Elfatih; Li, Xiaofen
PATENT ASSIGNEE(S): Cv Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 81 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004016635	A2	20040226	WO 2003-US25629	2003 0815
WO 2004016635	A3	20040408		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK,

MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU,
SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA,
UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,
DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL,
PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
GQ, GW, ML, MR, NE, SN, TD, TG

CA 2495370	AA	20040226	CA 2003-2495370	2003 0815
AU 2003263846	A1	20040303	AU 2003-263846	2003 0815
US 2004043960	A1	20040304	US 2003-641930	2003 0815
US 7022681	B2	20060404		
EP 1537133	A2	20050608	EP 2003-788541	2003 0815

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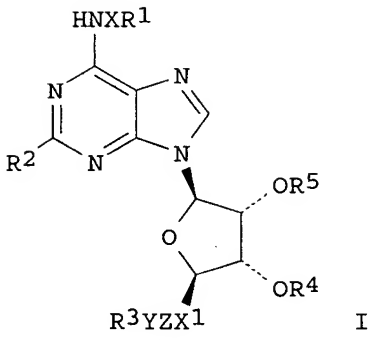
EE, HU, SK

CN 1675235	A	20050928	CN 2003-819361	2003 0815
JP 2006505525	T2	20060216	JP 2004-529472	2003 0815
NO 2005001296	A	20050513	NO 2005-1296	2005 0314
US 2006135467	A1	20060622	US 2006-355656	2006 0215

PRIORITY APPLN. INFO.:	US 2002-403712P	P	2002 0815
	US 2003-450094P	P	2003 0225
	US 2003-641930	A1	2003 0815
	WO 2003-US25629	W	2003 0815

OTHER SOURCE(S): MARPAT 140:199640
GI



I

AB Disclosed are novel compds. nucleosides I, wherein R1 is optionally substituted cycloalkyl, optionally substituted heterocyclyl, optionally substituted aryl, or optionally substituted heteroaryl; R2 is hydrogen, halo, trifluoromethyl, or cyano; R3 is hydrogen, optionally substituted cycloalkyl, optionally substituted aryl, optionally substituted heteroaryl, or optionally substituted heterocyclyl, R4 and R5 are independently hydrogen or optionally substituted acyl; X is a covalent bond or lower alkylene optionally substituted by cycloalkyl; X1 is a covalent bond or alkylene; Y is a covalent bond or lower alkylene optionally substituted by hydroxy or cycloalkyl; and Z is -C.tplbond.C-, alkenyl, alkyl, that are partial and full A1 adenosine receptor agonists, useful for treating various disease states, in particular the supraventricular tachycardias, emesis, angina, myocardial infarction and hyperlipidemia. Wherein the disease state is chosen from atrial fibrillation, supraventricular tachycardias and atrial flutter, congestive heart failure, epilepsy, stroke, diabetes, obesity, ischemia, stable angina, unstable angina, cardiac transplant, and myocardial infarction. Wherein the metabolic disorder is hyperlipidemia, non-insulin-dependent diabetes mellitus, or obesity. Thus, (4S,2R,3R,5R)-2-[6-(oxolan-3-yL-amino)purin-9-yl]-5-ethynyloxolane-3,4-diol was prepared and tested in rats as partial and full agonists of A1 adenosine receptor. Oral administration of (4S,2R,3R,5R)-2-[6-(cyclopentylamino)purin-9-yl]-5-[2-(2-fluorophenyl)ethynyl]oxolane-3,4-diol at a dose level of 1 mg/Kg provided an initial 40 % reduction of nonesterified free fatty acid (NEFA) that was maintained for 1 h, after which time the plasma levels of NEFA returned to normal in 2 h. Oral administration of (4S,2R,3R,5R)-2-[6-(cyclopentylamino)purin-9-yl]-5-[2-(2-fluorophenyl)ethynyl]oxolane-3,4-diol at a dose level of 2.5 mg/Kg provided an initial 60 % reduction of nonesterified free fatty acid (NEFA) that was maintained for 90 min, after which time the plasma levels of NEFA returned to normal in 4 h. At dose levels of 1 mg/Kg, 2.5 mg/Kg, and 5 mg/Kg, no effect on heart rate was observed

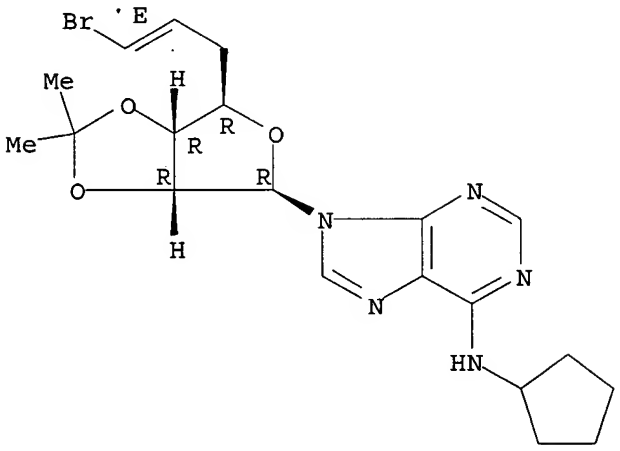
IT **661487-87-2P**
(preparation of adenosine derivs. as partial and full agonists of a adenosine receptors)

RN 661487-87-2 HCAPLUS

CN 9H-Purin-6-amine, 9-[(6E)-7-bromo-5,6,7-trideoxy-2,3-O-(1-methylethylidene)-β-D-ribo-hept-6-enofuranosyl]-N-cyclopentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

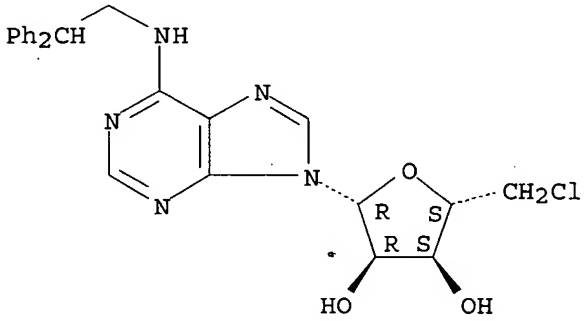


IC ICM C07H019-00
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT 458566-38-6P **661487-87-2P** 661487-88-3P 661487-89-4P
661487-90-7P 661487-91-8P 661487-92-9P 661487-93-0P
661487-94-1P 661487-95-2P
(preparation of adenosine derivs. as partial and full agonists of a adenosine receptors)

L40 ANSWER 4 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:178448 HCAPLUS
DOCUMENT NUMBER: 138:354164
TITLE: Solid-Phase Synthesis of Nucleoside Analogs
AUTHOR(S): Epple, Robert; Kudirka, Romas; Greenberg, William A.
CORPORATE SOURCE: Genomics Institute of the Novartis Research Foundation, San Diego, CA, 92121, USA
SOURCE: Journal of Combinatorial Chemistry (2003), 5(3), 292-310
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:354164
AB The synthesis of a 25 000 member library of nucleoside analogs as discrete compds. in milligram quantities is described. The use of the Nanokan technol. developed by IRORI (Discovery Partners International) together with macroporous solid support allowed us to develop a highly reliable and practical synthetic route for the high-throughput derivatization of both the pyrimidine and purine nucleoside scaffold. A 2',3'-acetal linkage of the scaffolds to the solid support proved to be stable enough for the chemical transformations employed, yet labile enough for mild cleavage conditions to yield final products in high purity. The publication represents an example for combining synthetic organic chemical on advanced scaffolds with the latest technologies of combinatorial chemical in order to provide both industrial and academic institutions with compds. in high number and quality, thereby accelerating the search for novel biol. targets and drug development.

IT **103626-52-4P**
(solid phase and combinatorial library synthesis of nucleoside analogs)
RN 103626-52-4 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(2,2-diphenylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-9 (Carbohydrates)
IT **103626-52-4P** 518315-87-2P 518315-90-7P 518315-91-8P
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518316-08-0P 518316-09-1P 518316-10-4P 518316-11-5P
518316-12-6P 518316-13-7P 518316-14-8P 518316-15-9P
518316-16-0P 518316-17-1P 518316-18-2P 518316-19-3P
(solid phase and combinatorial library synthesis of nucleoside analogs)
REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 5 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:319864 HCAPLUS
DOCUMENT NUMBER: 134:340357
TITLE: Novel compounds, specifically aromatic and heteroaromatic ureas and thioureas, useful against parasites and especially against coccidiosis.
INVENTOR(S): Muzi, Sabrina; Abdul-Rahman, Shoaa
PATENT ASSIGNEE(S): New Pharma Research Sweden AB, Swed.
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001030749	A1	20010503	WO 2000-SE2091	2000 1027

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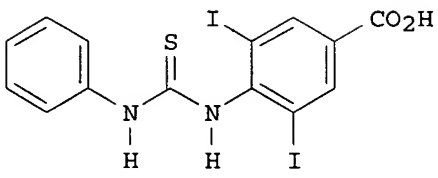
OTHER SOURCE(S): MARPAT 134:340357
GI



II

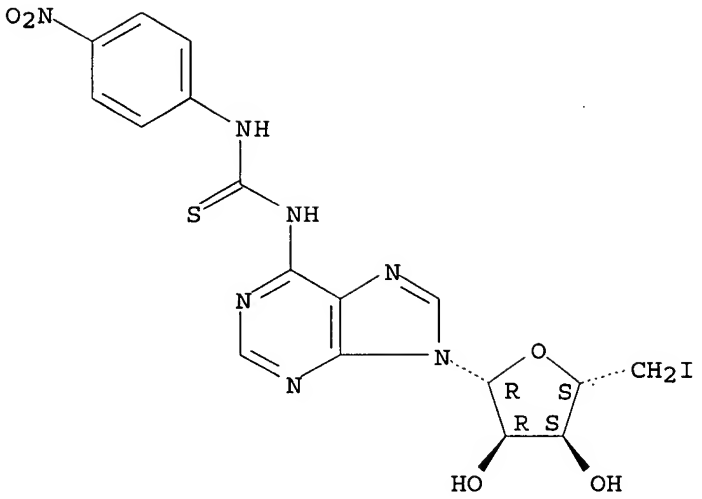
AB The invention relates to novel ureas and thioureas R-C(:Y)-R [I; Y = O or S; R's are selected from the pairings: (a) NHR1 and NHR2, or (b) NR3R4 and NR5R6, or (c) NR3R4 and cyclic radical -N:Z-R7; R1, R2 = certain (un)substituted aryl, aralkyl, alkyl, heteroaryl, etc.; R3-R6 = certain (un)substituted aryl, aralkyl, or alkyl groups; Z = atoms to form ring; R7 = electron-withdrawing substituent] and their tautomers, solvates, radiolabeled derivs., and pharmaceutically acceptable salts. Also disclosed are pharmaceutical compns. containing I, as well as a method for treatment of parasitic disorders using I. I are especially well-suited for treatment of coccidiosis, particularly in poultry. Over 200 compds. are listed, and several synthetic examples are given. For instance, reaction of PhNCS with 4-amino-3,5-diiodobenzoic acid in refluxing acetone in the presence of aqueous 10% KOH gave 75% thiourea derivative II. This compound had an anticoccidial effect in chickens similar to coxistac, but with a shorter duration of infection, reduced feed consumption, and no loss of growth rate.

IT **337531-62-1P**, N-[9-[3,4-Dihydroxy-5-(iodomethyl)tetrahydro-2-furanyl]-9H-purin-6-yl]-N'-(4-nitrophenyl)thiourea
(parasiticide candidate; preparation of aromatic and heteroarom. ureas and thioureas as antiparasitic and anticoccidial agents)

RN 337531-62-1 HCAPLUS

CN Adenosine, 5'-deoxy-5'-iodo-N-[[(4-nitrophenyl)amino]thioxomethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07C275-28
ICS C07D277-82; C07D295-16; A61K031-17; A61K031-425; A61K031-495; A61P033-02

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 5, 18, 27, 28

IT 370-52-5P, N-[4-Chloro-3-(trifluoromethyl)phenyl]-N'-(4-nitrophenyl)urea 3460-59-1P, N-(4-Cyanophenyl)-N'-phenylthiourea 20885-52-3P, N-(5-Chloro-2-pyridinyl)-N'-(4-nitrophenyl)urea 23747-76-4P, N-(4-Nitrophenyl)-N'-[4-(trifluoromethyl)phenyl]urea 32767-52-5P, N-[4-(Dimethylamino)phenyl]-N'-(4-nitrophenyl)thiourea 36726-57-5P, N-Phenyl-N'-(4-pyridinylmethyl)thiourea 57723-02-1P, N-[2-(4-Morpholinyl)ethyl]-N'-phenylthiourea 69194-88-3P, 3-[[(4-Nitroanilino)carbonyl]amino]benzoic acid 71196-82-2P, N-(5-Nitro-1,3-thiazol-2-yl)-N'-phenylthiourea 94000-66-5P, N-[4-(Dimethylamino)phenyl]-N'-(4-nitrophenyl)urea 309942-73-2P, N-Phenyl-N'-(tetrahydro-2-furanylmethyl)thiourea 316151-41-4P, N-(4-Cyanophenyl)-N'-(4-fluorophenyl)thiourea 321690-01-1P, N-(6-Nitro-1,3-benzothiazol-2-yl)-N'-phenylthiourea 330830-99-4P, N-(5-Methyl-1,3-thiazol-2-yl)-N'-phenylthiourea 337531-19-8P, N-(6-Nitro-1,3-benzothiazol-2-yl)-N'-(4-nitrophenyl)urea 337531-20-1P, 5-[(Anilinocarbothioyl)amino]isophthalic acid 337531-21-2P, 5-[[(4-Nitroanilino)carbothioyl]amino]isophthalic acid 337531-22-3P, N-(6-Nitro-1,3-benzothiazol-2-yl)-N'-(4-nitrophenyl)thiourea 337531-23-4P, N-(4-Fluorophenyl)-N'-(6-nitro-1,3-benzothiazol-2-yl)thiourea 337531-24-5P, N-Phenyl-N'-(3,4,5-trimethoxyphenyl)thiourea 337531-25-6P, 4-[(Anilinocarbothioyl)amino]-3,5-diiodobenzoic acid 337531-26-7P, 4-[[[(Carboxymethyl)amino]carbothioyl]amino]-3,5-diiodobenzoic acid 337531-27-8P, 4-[[[(2,3-Diiodopropyl)amino]carbothioyl]amino]-3,5-diiodobenzoic acid 337531-28-9P, N-(4-Cyanophenyl)-N'-(4-nitrophenyl)thiourea 337531-29-0P, N-[2-(4-Morpholinyl)ethyl]-N'-(4-nitrophenyl)thiourea 337531-30-3P, N-[2-[(4-Nitrophenyl)sulfonyl]-1,3-thiazol-5-yl]-N'-phenylthiourea 337531-31-4P, (2S,5R)-3,3-Dimethyl-6-[[(4-nitroanilino)carbothioyl]amino]-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid 337531-32-5P,

1-[[(4-Nitroanilino)carbonyl]amino]cyclopentanecarboxylic acid 337531-33-6P, 4-[[[(4-Nitroanilino)carbonyl]amino]methyl]cyclohexanecarboxylic acid 337531-34-7P, 4-[[(4-Nitroanilino)carbonyl]amino]cyclohexanecarboxylic acid 337531-35-8P, 3-[[(4-Nitroanilino)carbothioyl]amino]benzoic acid 337531-36-9P, N-(4-Nitrophenyl)-N'-[4-nitro-2-(trifluoromethyl)phenyl]urea 337531-37-0P, N-(4-Nitrophenyl)-N'-[2-nitro-4-(trifluoromethyl)phenyl]urea 337531-38-1P, 2,3,6-Trifluoro-5-[[(4-nitroanilino)carbonyl]amino]benzoic acid 337531-39-2P, 2,3,6-Trifluoro-5-[[(4-nitroanilino)carbothioyl]amino]benzoic acid 337531-40-5P, N-(2,5-Dicyano-3,4,6-trifluorophenyl)-N'-(4-nitrophenyl)thiourea 337531-41-6P, N-(2,5-Dicyano-3,4,6-trifluorophenyl)-N'-(4-nitrophenyl)urea 337531-42-7P, N-(3-Chloro-2,5,6-trifluoro-4-pyridinyl)-N'-(4-nitrophenyl)urea 337531-43-8P, N-(4-Nitrophenyl)-N'-(2,2,2-trifluoroethyl)urea 337531-44-9P, N-(4-Nitrophenyl)-N'-(2,2,2-trifluoroethyl)thiourea 337531-45-0P, N-(2-Benzoyl-4-iodophenyl)-N'-(4-nitrophenyl)urea 337531-46-1P, N-(2-Benzoyl-4-iodophenyl)-N'-(4-nitrophenyl)thiourea 337531-48-3P, N-[3-(4-Iodophenyl)-1,4-dioxo-1,4-dihydro-2-naphthalenyl]-N'-(4-nitrophenyl)thiourea 337531-50-7P, N-[3-(4-Iodophenyl)-1,4-dioxo-1,4-dihydro-2-naphthalenyl]-N'-(4-nitrophenyl)urea 337531-52-9P, 4-Iodo-N-[(4-nitroanilino)carbothioyl]phenylalanine 337531-53-0P, 4-Iodo-N-[(4-nitroanilino)carbonyl]phenylalanine 337531-54-1P, N-[1-[3,4-Dihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]-5-iodo-2-oxo-1,2-dihydro-4-pyrimidinyl]-N'-(4-nitrophenyl)urea 337531-55-2P, N-[1-[3,4-Dihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]-5-iodo-2-oxo-1,2-dihydro-4-pyrimidinyl]-N'-(4-nitrophenyl)thiourea 337531-56-3P, 4-(4-Hydroxy-3-iodophenoxy)-3,5-diiodo-N-[(4-nitroanilino)carbothioyl]phenylalanine 337531-57-4P, 4-(4-Hydroxy-3-iodophenoxy)-3,5-diiodo-N-[(4-nitroanilino)carbonyl]phenylalanine 337531-58-5P, 4-Hydroxy-3-iodo-N-[(4-nitroanilino)carbonyl]phenylalanine 337531-59-6P, 3-(4-Hydroxy-3-iodophenyl)-2-[[(4-nitroanilino)carbonyl]amino]propanethioic O-acid 337531-60-9P, 5-Iodo-2-[[(4-nitroanilino)carbonyl]amino]benzoic acid 337531-61-0P, N-[9-[3,4-Dihydroxy-5-(iodomethyl)tetrahydro-2-furanyl]-9H-purin-6-yl]-N'-(4-nitrophenyl)urea **337531-62-1P**, N-[9-[3,4-Dihydroxy-5-(iodomethyl)tetrahydro-2-furanyl]-9H-purin-6-yl]-N'-(4-nitrophenyl)thiourea 337531-63-2P, 3,5,6-Trichloro-4-[[(4-nitroanilino)carbonyl]amino]-2-pyridinecarboxylic acid 337531-64-3P, 3-[[(4-Nitroanilino)carbonyl]amino]-2-quinoxalinecarboxylic acid 337531-65-4P, 4-[[(4-Nitroanilino)carbonyl]amino]-2-quinolinecarboxylic acid 337531-66-5P, 4-[[(4-Nitroanilino)carbothioyl]amino]-2-quinolinecarboxylic acid 337531-67-6P, 4-[[(4-Nitroanilino)carbothioyl]amino]-5-pyrimidinecarboxylic acid 337531-68-7P, 3-[[(4-Nitroanilino)carbothioyl]amino]bicyclo[2.2.1]heptane-2-carboxylic acid 337531-69-8P, 4-[[[(4-Nitroanilino)carbothioyl]amino]methyl]cyclohexanecarboxylic acid 337531-70-1P, 6-Hydroxy-2-[[(4-nitroanilino)carbothioyl]amino]-4-pyrimidinecarboxylic acid 337531-71-2P, 5-Chloro-2-[[(4-nitroanilino)carbothioyl]amino]-4-pyrimidinecarboxylic acid 337531-72-3P, 1-[[(4-Nitroanilino)carbonyl]amino]-9,10-dioxo-9,10-dihydro-2-anthracenecarboxylic acid 337531-73-4P, 3-[[(4-Nitroanilino)carbonyl]amino]-1-adamantanecarboxylic acid 337531-74-5P, (1S,3R)-1-[[(4-Nitroanilino)carbonyl]amino]-1,3-cyclopentanedicarboxylic acid 337531-75-6P, 2-(Ethylsulfanyl)-4-

[[(4-nitroanilino)carbonyl]amino]-5-pyrimidinecarboxylic acid 337531-76-7P, 3-[[(4-Nitroanilino)carbonyl]amino]-1,1,3-propanetricarboxylic acid 337531-77-8P, 3-[[(4-Nitroanilino)carbonyl]amino]-2-pyrazinecarboxylic acid 337531-78-9P, 1-[[(4-Nitroanilino)carbonyl]amino]cyclopropanecarboxylic acid 337531-79-0P, 1-[[(4-Nitroanilino)carbothioyl]amino]cyclopropanecarboxylic acid 337531-80-3P, 2-[2,3,4-Trihydroxy-1-[1-[[(4-nitroanilino)carbonyl]amino]-2-oxoethyl]butoxy]propanoic acid 337531-81-4P, N-(4-Nitrophenyl)-N'-[4-oxo-6-((1R,2S)-1,2,3-trihydroxypropyl)-4,8-dihydro-2-pteridinyl]urea 337531-82-5P, N-(4-Nitrophenyl)-N'-(2,4,5-trihydroxyphenethyl)urea 337531-83-6P, 5-[[(4-Nitroanilino)carbonyl]amino]-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarboxylic acid 337531-84-7P, 1,3-Dihydroxy-4-[[(4-nitroanilino)carbonyl]amino]-9,10-dioxo-9,10-dihydro-2-anthracenesulfonic acid 337531-85-8P, 2,4,5-Trihydroxy-N-[(4-nitroanilino)carbonyl]phenylalanine 337531-86-9P, N-[1-[3,4-Dihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]-6-oxo-1,6-dihydro-4-pyrimidinyl]-N'-(4-nitrophenyl)urea 337531-87-0P, N-[(1R,2S)-2-(3,4-Dihydroxyphenyl)-2-hydroxy-1-methylethyl]-N'-(4-nitrophenyl)urea 337531-88-1P, N-(3,4-Dihydroxybenzyl)-N'-(4-nitrophenyl)urea 337531-89-2P, N-[1-[3,4-Dihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]-5-methyl-2-oxo-1,2-dihydro-4-pyrimidinyl]-N'-(4-nitrophenyl)urea 337531-90-5P, N-[1-[3,4-Dihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]-2-thioxo-1,2-dihydro-4-pyrimidinyl]-N'-(4-nitrophenyl)urea 337531-91-6P, N-[1-[3,4-Dihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]-2-oxo-1,2-dihydro-4-pyrimidinyl]-N'-(4-nitrophenyl)urea 337531-92-7P, N-[4,5-Dihydroxy-7-[[(4-nitroanilino)carbonyl]amino]-9,10-dioxo-9,10-dihydro-2-anthracenyl]-N'-(4-nitrophenyl)urea 337531-93-8P, N-(3,4-Dihydroxyphenethyl)-N'-(4-nitrophenyl)urea 337531-94-9P, N-[2-(3,4-Dihydroxyphenyl)-2-hydroxyethyl]-N'-(4-nitrophenyl)urea 337531-95-0P, 1-[[(4-Nitroanilino)carbonyl]amino]-1,3-cyclobutanedicarboxylic acid 337531-96-1P, (1R,3R)-1-[[(4-Nitroanilino)carbonyl]amino]-1,3-cyclopentanedicarboxylic acid 337531-97-2P, 2-[2-[[(4-Nitroanilino)carbonyl]amino]benzoyl]benzoic acid 337531-98-3P, 6-[[(4-Nitroanilino)carbonyl]amino]nicotinic acid 337531-99-4P, 1-[[(4-Nitroanilino)carbonyl]amino]cyclohexanecarboxylic acid 337532-00-0P, 2-[[(4-Nitroanilino)carbonyl]amino]bicyclo[2.2.1]heptane-2-carboxylic acid 337532-01-1P, N'-[2-[[(3-Nitroanilino)carbonyl]amino]ethyl]-N-(4-nitrophenyl)urea 337532-02-2P, N'-[2-[[(3-Nitroanilino)carbothioyl]amino]ethyl]-N-(4-nitrophenyl)thiourea 337532-03-3P, N'-[4-[[(3-Nitroanilino)carbonyl]amino]butyl]-N-(4-nitrophenyl)urea 337532-04-4P, N'-[4-[[(3-Nitroanilino)carbothioyl]amino]butyl]-N-(4-nitrophenyl)thiourea 337532-05-5P, N'-[4-[[(4-Nitroanilino)carbonyl]amino]phenyl]-N-(4-nitrophenyl)urea 337532-06-6P, N'-[4-[[(4-Nitroanilino)carbothioyl]amino]phenyl]-N-(4-nitrophenyl)thiourea 337532-07-7P, N'-[5-[[(3-Nitroanilino)carbonyl]amino]pentyl]-N-(4-nitrophenyl)urea 337532-08-8P, N'-[5-[[(3-Nitroanilino)carbothioyl]amino]pentyl]-N-(4-nitrophenyl)thiourea 337532-09-9P, 4,4'-Bis[[(4-nitroanilino)carbonyl]amino]-1,1'-biphenyl 337532-10-2P, 4,4'-Bis[[(4-nitroanilino)carbothioyl]amino]-1,1'-biphenyl 337532-11-3P, N-(4,5-Dihydroxy-2-pyrimidinyl)-N'-(4-nitrophenyl)urea 337532-12-4P, N-(4,5-Dihydroxy-2-pyrimidinyl)-N'-(4-nitrophenyl)thiourea 337532-13-5P, 3,3'-Dichloro-4,4'-bis[[(4-nitroanilino)carbonyl]amino]-1,1'-biphenyl 337532-14-6P, 3,3'-Dichloro-4,4'-bis[[(4-nitroanilino)carbothioyl]amino]-1,1'-

biphenyl 337532-15-7P, 3,3'-Dimethyl-4,4'-bis[[(4-nitroanilino)carbonyl]amino]-1,1'-biphenyl 337532-16-8P, 3,3'-Dimethyl-4,4'-bis[[(4-nitroanilino)carbothioyl]amino]-1,1'-biphenyl 337532-17-9P, N-[4-(Diethylamino)-1-methylbutyl]-N'-(4-nitrophenyl)urea 337532-18-0P, N-[4-(Diethylamino)-1-methylbutyl]-N'-(4-nitrophenyl)thiourea 337532-19-1P, N'-[6-[[(4-Nitroanilino)carbonyl]amino]-3-acridinyl]-N-(4-nitrophenyl)urea 337532-20-4P, N'-[6-[[(4-Nitroanilino)carbothioyl]amino]-3-acridinyl]-N-(4-nitrophenyl)thiourea 337532-21-5P, N-[2,4-Dibromo-6-[[cyclohexyl(methyl)amino]methyl]phenyl]-N'-(4-nitrophenyl)urea 337532-22-6P, N-[2,4-Dibromo-6-[[cyclohexyl(methyl)amino]methyl]phenyl]-N'-(4-nitrophenyl)thiourea 337532-23-7P, N-(6-Chloro-2-pyrazinyl)-N'-(4-nitrophenyl)urea 337532-24-8P, N-(6-Chloro-2-pyrazinyl)-N'-(4-nitrophenyl)thiourea 337532-25-9P, N-(5-Chloro-2-pyridinyl)-N'-(4-nitrophenyl)thiourea 337532-26-0P, N-[[2-[(E)-(2,6-Dichlorophenyl)methylidene]hydrazino](imino)methyl]-N'-(4-fluorophenyl)urea 337532-28-2P, N-[[2-[(E)-(2,6-Dichlorophenyl)methylidene]hydrazino](imino)methyl]-N'-(4-fluorophenyl)thiourea 337532-30-6P, 2-[[[[(4-Fluoroanilino)carbonyl]amino](imino)methyl]amino]acetic acid 337532-31-7P, 2-[[[[(4-Fluoroanilino)carbothioyl]amino](imino)methyl]amino]acetic acid 337532-32-8P, 2-[[[[[(4-Fluoroanilino)carbonyl]amino](imino)methyl]amino]methyl]-2,3-dihydro-1,4-benzodioxine 337532-33-9P, 2-[[[[[(4-Fluoroanilino)carbothioyl]amino](imino)methyl]amino]methyl]-2,3-dihydro-1,4-benzodioxine 337532-34-0P, 1-Fluoro-4-[[[[imino[(3-methyl-2-butenyl)amino]methyl]amino]carbonyl]amino]benzene 337532-35-1P, 1-Fluoro-4-[[[[imino[(3-methyl-2-butenyl)amino]methyl]amino]carbothioyl]amino]benzene 337532-36-2P, 2-[[[[[(4-Fluoroanilino)carbonyl]amino](imino)methyl]amino]methyl]-1,4-dioxaspiro[4.5]decane 337532-37-3P, 2-[[[[[(4-Fluoroanilino)carbothioyl]amino](imino)methyl]amino]methyl]-1,4-dioxaspiro[4.5]decane 337532-38-4P, 1,3-Dichloro-2-[1-[[[[(4-fluoroanilino)carbonyl]amino](imino)methyl]amino]-2-oxoethyl]benzene 337532-39-5P, 1,3-Dichloro-2-[1-[[[[(4-fluoroanilino)carbothioyl]amino](imino)methyl]amino]-2-oxoethyl]benzene 337532-40-8P, 1-[[[[(Cyanoamino)(imino)methyl]amino]carbonyl]amino]-4-fluorobenzene 337532-41-9P, 1-[[[[(Cyanoamino)(imino)methyl]amino]carbothioyl]amino]-4-fluorobenzene 337532-42-0P, N'-[[[(4-Fluoroanilino)carbonyl]amino](imino)methyl]-N-(4-fluorophenyl)urea 337532-43-1P, N'-[[[(4-Fluoroanilino)carbothioyl]amino](imino)methyl]-N-(4-fluorophenyl)thiourea 337532-44-2P, 1-Fluoro-4-[[[[[[3-[[[[(4-fluoroanilino)carbonyl]amino](imino)methyl]amino]-2,4,5,6-tetrahydroxycyclohexyl]amino](imino)methyl]amino]carbonyl]amino]benzene 337532-45-3P, 1-Fluoro-4-[[[[[[3-[[[[(4-fluoroanilino)carbothioyl]amino](imino)methyl]amino]-2,4,5,6-tetrahydroxycyclohexyl]amino](imino)methyl]amino]carbothioyl]amino]benzene 337532-46-4P, N-(4-Fluorophenyl)-N'-[imino[2-[(E)-3-(5-nitro-2-furyl)-1-[(E)-2-(5-nitro-2-furyl)ethenyl]-2-propenylidene]hydrazino]methyl]urea 337532-47-5P, N-(4-Fluorophenyl)-N'-[imino[2-[(E)-3-(5-nitro-2-furyl)-1-[(E)-2-(5-nitro-2-furyl)ethenyl]-2-propenylidene]hydrazino]methyl]thiourea 337532-48-6P, N,N'-Bis(5-bromo-2-pyridinyl)-N-(6-nitro-1,3-benzothiazol-2-yl)-N'-(4-nitrophenyl)urea 337532-49-7P, N,N'-Bis(6-chloro-2-pyrazinyl)-N-(6-nitro-1,3-benzothiazol-2-yl)-N'-(4-nitrophenyl)thiourea 337532-50-0P, N,N'-Bis(6-chloro-2-pyridinyl)-N-(6-nitro-1,3-benzothiazol-2-yl)-N'-(4-nitrophenyl)urea 337532-51-1P, 4-Nitro-N-(6-nitro-1,3-

benzothiazol-2-yl)-N-[[N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]benzenesulfonamide 337532-52-2P, 4-Nitro-N-(6-nitro-1,3-benzothiazol-2-yl)-N-[[4-nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]benzenesulfonamide 337532-53-3P, 4-Nitro-N-(6-nitro-1,3-benzothiazol-2-yl)-N-[[4-nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbonyl]benzenesulfonamide 337532-54-4P, 5-[[[4-Nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl][(4-nitrophenyl)sulfonyl]amino]isophthalic acid 337532-55-5P, 5-[[[4-Fluoro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl][(4-nitrophenyl)sulfonyl]amino]isophthalic acid 337532-56-6P, 5-[N-(6-Bromo-2-pyridinyl)-N-[[N-(5-bromo-2-pyridinyl)-4-fluoroanilino]carbothioyl]amino]isophthalic acid 337532-57-7P, 5-[N-(6-Chloro-2-pyrazinyl)-N-[[N-(6-chloro-2-pyrazinyl)-4-fluoroanilino]carbothioyl]amino]isophthalic acid 337532-58-8P, 5-[N-(6-Chloro-2-pyridinyl)-N-[[N-(6-chloro-2-pyridinyl)-4-fluoroanilino]carbothioyl]amino]isophthalic acid 337532-59-9P, 5-[N-(6-Chloro-2-pyridinyl)-N-[[N-(6-chloro-2-pyridinyl)-4-nitroanilino]carbothioyl]amino]isophthalic acid 337532-60-2P, N-(4-Fluorophenyl)-4-nitro-N-[[(6-nitro-1,3-benzothiazol-2-yl)[(4-nitrophenyl)sulfonyl]amino]carbothioyl]benzenesulfonamide 337532-61-3P, N,N'-Bis(6-chloro-2-pyrazinyl)-N-(4-fluorophenyl)-N'-(6-nitro-1,3-benzothiazol-2-yl)thiourea 337532-62-4P, N,N'-Bis(6-chloro-2-pyridinyl)-N-(4-fluorophenyl)-N'-(6-nitro-1,3-benzothiazol-2-yl)thiourea 337532-63-5P, 4-[[[(1,3-Benzothiazol-2-yl)[(4-nitrophenyl)sulfonyl]amino]carbothioyl][(4-nitrophenyl)sulfonyl]amino]phthalic acid 337532-64-6P, 4-[[[4-[[[(6-Nitro-1,3-benzothiazol-2-yl)[(4-nitrophenyl)sulfonyl]amino]carbothioyl][(4-nitrophenyl)sulfonyl]amino]phenyl]sulfonyl]amino]benzoic acid 337532-65-7P, N-(1,3-Benzothiazol-2-yl)-N-[[(8-chloro-5-quinolinyl)[(4-nitrophenyl)sulfonyl]amino]carbothioyl]-4-nitrobenzenesulfonamide 337532-66-8P, N-(8-Chloro-5-quinolinyl)-N-[[(8-chloro-5-quinolinyl)[(4-nitrophenyl)sulfonyl]amino]carbothioyl]-4-nitrobenzenesulfonamide 337532-67-9P, N-[[(6-Chloro-2-pyrazinyl)[(4-fluorophenyl)sulfonyl]amino]carbothioyl]-N-(3-chloro-4-pyridinyl)-4-fluorobenzenesulfonamide 337532-68-0P, N-(3-Chloro-4-pyridinyl)-4-fluoro-N-[[N-[(4-fluorophenyl)sulfonyl]-3-(trifluoromethyl)anilino]carbothioyl]benzenesulfonamide 337532-69-1P, N-[[4-Fluoro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-N-[(4-methylphenyl)sulfonyl]-4-nitrobenzenesulfonamide 337532-70-4P, N-[[5-(Dimethylamino)-1-naphthyl]sulfonyl]-N-[[4-fluoro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-4-nitrobenzenesulfonamide 337532-71-5P, N-[(7-Fluoro-2,1,3-benzoxadiazol-4-yl)sulfonyl]-N-[[4-fluoro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-4-nitrobenzenesulfonamide 337532-72-6P, N-[[4-Fluoro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-N-[(6-methyl-1,1-dioxo-1,2,3,4-tetrahydrothiochromen-7-yl)sulfonyl]-4-nitrobenzenesulfonamide 337532-73-7P, N-[[(6-Nitro-1,3-benzothiazol-2-yl)(phenylsulfonyl)amino]carbothioyl]-N-(3-nitrophenyl)benzenesulfonamide 337532-74-8P, 3,5-Diiodo-4-[N-[(4-nitrophenyl)sulfonyl]-N-[[N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]amino]benzoic acid 337532-75-9P, 4-[N-[(4-Fluorophenyl)sulfonyl]-N-[[N-[(4-fluorophenyl)sulfonyl]anilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-76-0P, 4-[N-[(4-Fluorophenyl)sulfonyl]-N-[[N-[(4-fluorophenyl)sulfonyl]-4-nitroanilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-77-1P, 3,5-Diiodo-4-[[[4-nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl][(4-

nitrophenyl)sulfonyl]amino]benzoic acid 337532-78-2P, 4-[[[4-Fluoro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl][(4-nitrophenyl)sulfonyl]amino]-3,5-diiodobenzoic acid 337532-79-3P, 4-[N-(5-Bromo-2-pyridinyl)-N-[[N-(5-bromo-2-pyridinyl)anilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-80-6P, 4-[N-(6-Chloro-2-pyrazinyl)-N-[[N-(6-chloro-2-pyrazinyl)anilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-81-7P, 4-[N-(6-Chloro-2-pyrazinyl)-N-[[N-(6-chloro-2-pyrazinyl)-4-nitroanilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-82-8P, 3,5-Diiodo-4-[N-[[4-nitro-N-(2-pyrazinyl)anilino]carbothioyl]-N-(2-pyrazinyl)amino]benzoic acid 337532-83-9P, 4-[N-[[4-Fluoro-N-(2-pyrazinyl)anilino]carbothioyl]-N-(2-pyrazinyl)amino]-3,5-diiodobenzoic acid 337532-84-0P, 4-[N-(6-Chloro-2-pyrazinyl)-N-[[N-(6-chloro-2-pyrazinyl)-4-fluoroanilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-85-1P, 4-[N-(6-Chloro-2-pyridinyl)-N-[[N-(6-chloro-2-pyridinyl)-4-fluoroanilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-86-2P, 4-[N-(6-Chloro-2-pyridinyl)-N-[[N-(6-chloro-2-pyridinyl)-4-nitroanilino]carbothioyl]amino]-3,5-diiodobenzoic acid 337532-87-3P, 4-[[[N-(Carboxymethyl)-N-[(trifluoromethyl)sulfonyl]amino]carbothioyl]-N-[(trifluoromethyl)sulfonyl]amino]-3,5-diiodobenzoic acid 337532-88-4P, 3,5-Diiodo-4-[N-(2-naphthylsulfonyl)-N-[[N-(2-naphthylsulfonyl)-N-(phenethyl)amino]carbothioyl]amino]benzoic acid 337532-89-5P, 4-[N-[[4-Carboxy-3-hydroxy-N-(2-naphthylsulfonyl)anilino]carbothioyl]-N-(2-naphthylsulfonyl)amino]-3,5-diiodobenzoic acid 337532-90-8P, 4-[[[(2,3-Diiodopropyl)[(4-nitrophenyl)sulfonyl]amino]carbothioyl][(4-nitrophenyl)sulfonyl]amino]-3,5-diiodobenzoic acid 337532-91-9P, N-(5-Chloro-2-pyridinyl)-N'-(6-chloro-2-pyridinyl)-N'-(4-cyanophenyl)-N-(4-nitrophenyl)thiourea 337532-92-0P, N,N'-Bis(6-chloro-2-pyrazinyl)-N-(4-cyanophenyl)-N'-(4-nitrophenyl)thiourea 337532-93-1P, N,N'-Bis(5-bromo-2-pyridinyl)-N-(4-cyanophenyl)-N'-(4-nitrophenyl)thiourea 337532-94-2P, N-[[4-Cyano-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-4-nitro-N-(4-nitrophenyl)benzenesulfonamide 337532-95-3P, N-(4-Cyanophenyl)(trifluoro)-N-[[4-nitro-N-[(trifluoromethyl)sulfonyl]anilino]carbothioyl]methanesulfonamide 337532-96-4P, N-(4-Cyanophenyl)trifluoro-N-[[4-fluoro-N-[(trifluoromethyl)sulfonyl]anilino]carbothioyl]methanesulfonamide 337532-97-5P, 4-Nitro-N-[[N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-N-(3,4,5-trimethoxyphenyl)benzenesulfonamide 337532-98-6P, N-[[4-Isopropyl-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-4-nitro-N-(4-nitrophenyl)benzenesulfonamide 337532-99-7P, N,N'-Bis(3-chloro-2-pyridinyl)-N-[2-(4-morpholinyl)ethyl]-N'-(4-nitrophenyl)thiourea 337533-00-3P, N,N'-Bis(6-chloro-2-pyrazinyl)-N-[2-(4-morpholinyl)ethyl]-N'-(4-nitrophenyl)thiourea 337533-01-4P, N-[2-(4-Morpholinyl)ethyl]-4-nitro-N-[[4-nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]benzenesulfonamide 337533-02-5P, Trifluoro-N-[2-(4-morpholinyl)ethyl]-N-[[4-nitro-N-[(trifluoromethyl)sulfonyl]anilino]carbothioyl]methanesulfonamide 337533-03-6P, 1-[[[4-Nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbonyl][(4-nitrophenyl)sulfonyl]amino]cyclopentanecarboxylic acid 337533-04-7P, 3-[[[4-Nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbonyl][(4-nitrophenyl)sulfonyl]amino]benzoic acid 337533-05-8P, 4-Nitro-N-[[4-nitro-N-[(4-nitrophenyl)sulfonyl]-2-(trifluoromethyl)anilino]carbonyl]-N-(4-nitrophenyl)benzenesulfonamide 337533-06-9P, 4-Fluoro-N-[[N-[(4-fluorophenyl)sulfonyl]-2-nitro-4-

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isoquinolinyl]ethyl]-N-[(4-nitrophenyl)sulfonyl]benzenesulfonamide 337533-31-0P, N-(1-Azepanyl)-N-[[[[4-[2-[[(5-methyl-3-isoxazolyl)carbonyl][(4-nitrophenyl)sulfonyl]amino]ethyl]phenyl]sulfonyl][(4-nitrophenyl)sulfonyl]amino]carbonyl]-4-nitrobenzenesulfonamide 337533-33-2P, [N-[[N-(3-Hydroxy-4,7,7-trimethylbicyclo[2.2.1]hept-2-yl)-4-nitroanilino]carbonyl]-4-nitroanilino](4-methylphenyl)dioxosulfane 337533-35-4P, N-Butyl-4-nitro-N-[[N-[(4-nitrophenyl)sulfonyl]-N-[[4-[[(4-nitrophenyl)sulfonyl]amino]phenyl]sulfonyl]amino]carbonyl]benzenesulfonamide 337533-37-6P, N-[[Cyclohexyl[(4-nitrophenyl)sulfonyl]amino]carbonyl]-N-(2,3-dihydro-1H-inden-5-ylsulfonyl)-4-nitrobenzenesulfonamide 337533-39-8P, N,N'-Bis(4-nitrophenyl)-1,4-piperazinedicarbothioamide 337533-41-2P, 4-Nitro-N-[[4-[[4-nitro-N-[(4-nitrophenyl)sulfonyl]anilino]carbothioyl]-1-piperazinyl]carbothioyl]-N-(4-nitrophenyl)benzenesulfonamide
(parasiticide candidate; preparation of aromatic and heteroarom. ureas and thioureas as antiparasitic and anticoccidial agents)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 1999:325951 HCAPLUS
DOCUMENT NUMBER: 130:325349
TITLE: Preparation of nucleosides as adenosine A1 receptors
INVENTOR(S): Box, Philip Charles; Judkins, Brian David; Pennell, Andrew Michael Kenneth
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 53 pp.
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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			WO 1998-EP7022 W	1998 1106

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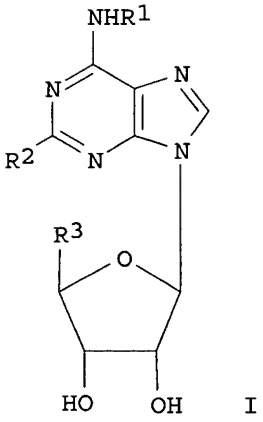


I

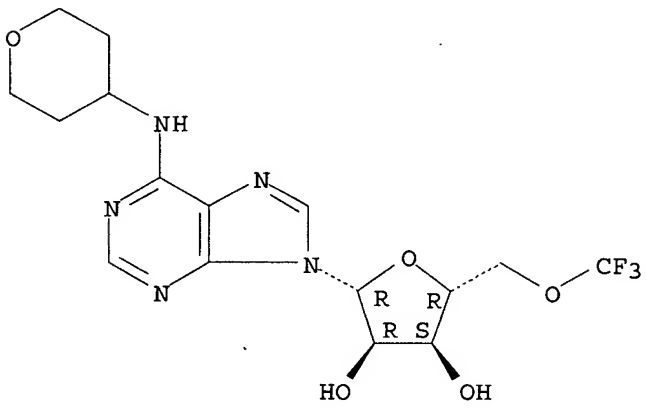
AB Deoxyfluoro nucleosides I which are agonists at the adenosine A1 receptor wherein R1 represents cycloalkyl, heterocylic,alkyl, bicyclic heterocycle, aryl; R2 represents C1-3 alkyl, halogen or hydrogen; R3 represents a fluorinated straight or branched O-alkyl group of 1-6 carbon atoms and salts and solvates thereof, in particular, physiol. acceptable solvates and salts thereof. These compds. are agonists at the Adenosine A1 receptor. Thus, N-(tetrahydro-pyran-4-yl)-5'-O-trifluoromethyladenosine was prepared and tested as adenosine A1 receptor (equipotent concentration ratio relative to NECA = 8.40).

IT **223761-50-0P 223761-51-1P 223761-53-3P**
223761-54-4P 223761-55-5P 223761-56-6P
223761-57-7P 223761-58-8P 223761-59-9P
223761-60-2P 223761-61-3P 223761-62-4P
223761-63-5P 223761-64-6P 223761-65-7P
223761-67-9P 223761-68-0P 223761-69-1P
223761-70-4P 223761-73-7P 223761-74-8P
223919-49-1P
(preparation of nucleosides as adenosine A1 receptors)

RN 223761-50-0 HCAPLUS

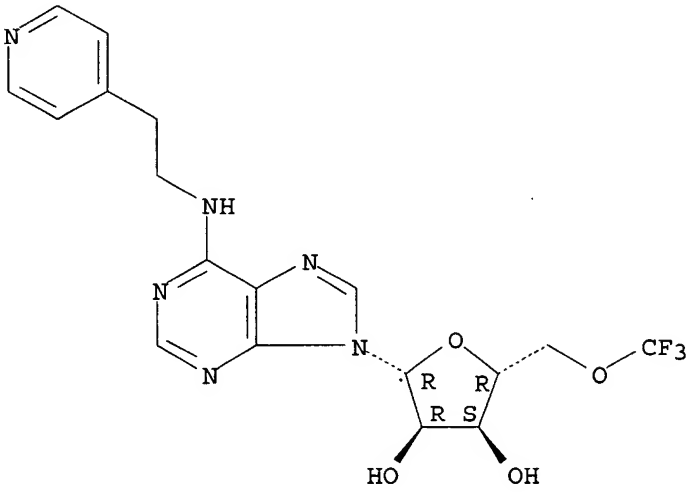
CN Adenosine, N-(tetrahydro-2H-pyran-4-yl)-5'-O-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



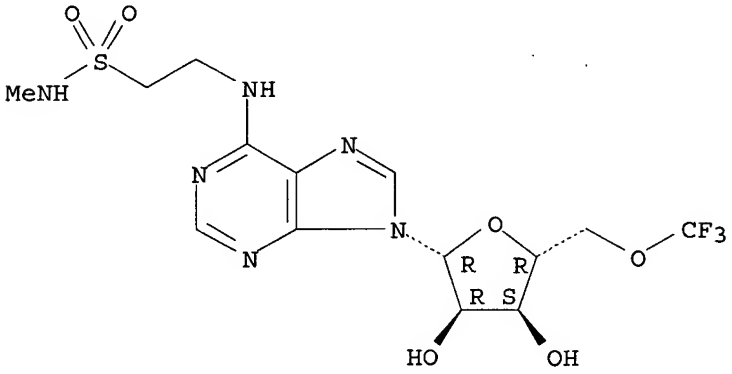
RN 223761-51-1 HCAPLUS
CN Adenosine, N-[2-(4-pyridinyl)ethyl]-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



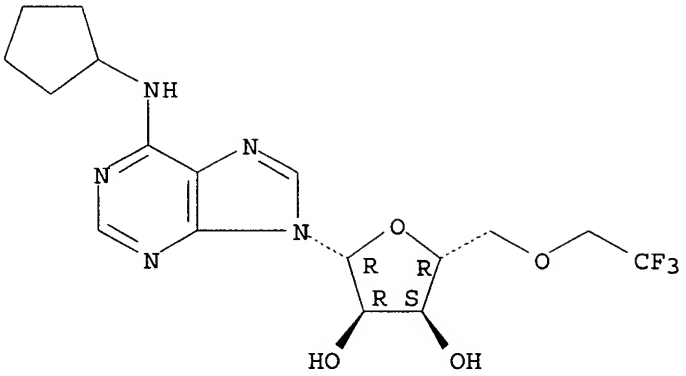
RN 223761-53-3 HCAPLUS
CN Adenosine, N-[2-[(methylamino)sulfonyl]ethyl]-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



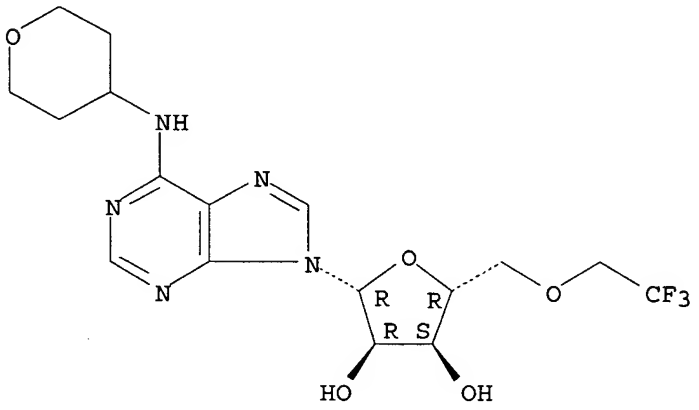
RN 223761-54-4 HCAPLUS
CN Adenosine, N-cyclopentyl-5'-O-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



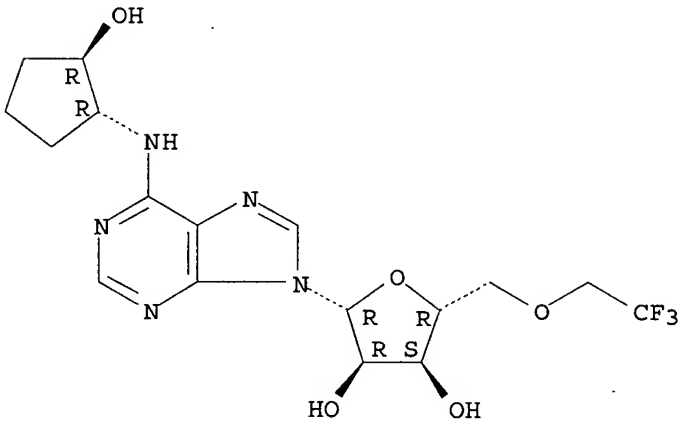
RN 223761-55-5 HCAPLUS
CN Adenosine, N-(tetrahydro-2H-pyran-4-yl)-5'-O-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



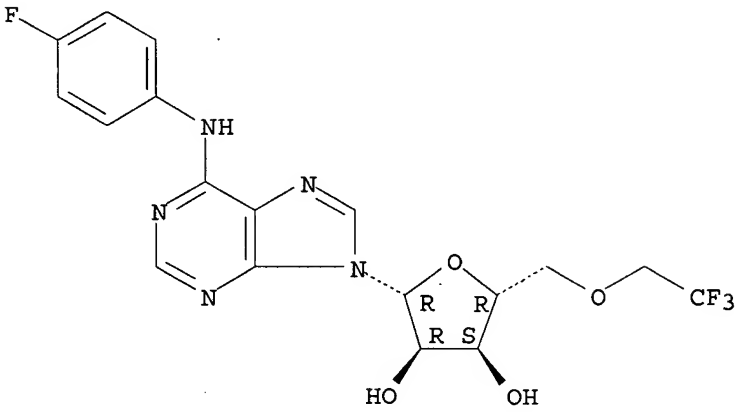
RN 223761-56-6 HCAPLUS
CN Adenosine, N-[(1R,2R)-2-hydroxycyclopentyl]-5'-O-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



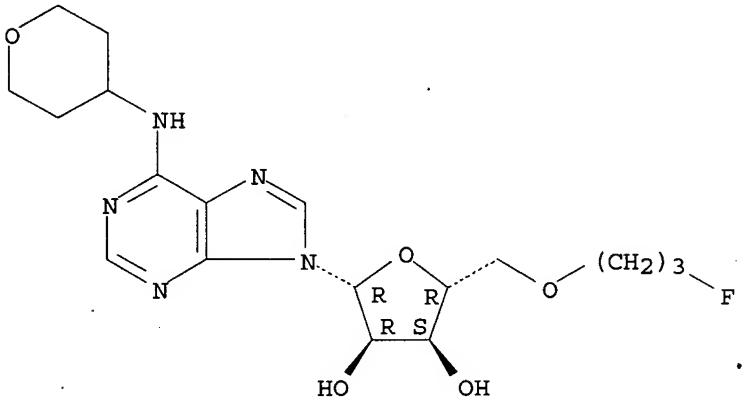
RN 223761-57-7 HCAPLUS
CN Adenosine, N-(4-fluorophenyl)-5'-O-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



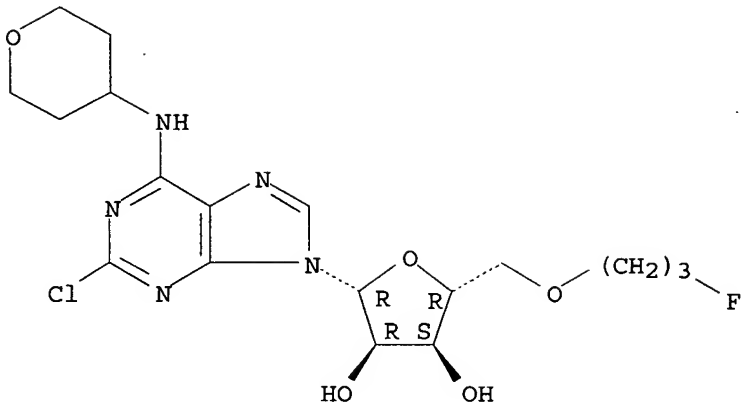
RN 223761-58-8 HCAPLUS
CN Adenosine, 5'-O-(3-fluoropropyl)-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



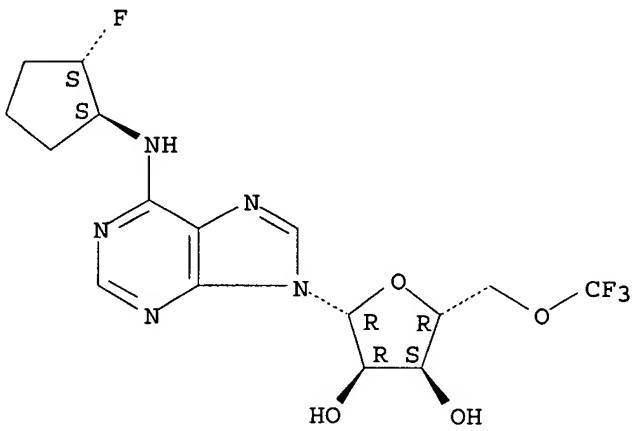
RN 223761-59-9 HCAPLUS
CN Adenosine, 2-chloro-5'-O-(3-fluoropropyl)-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



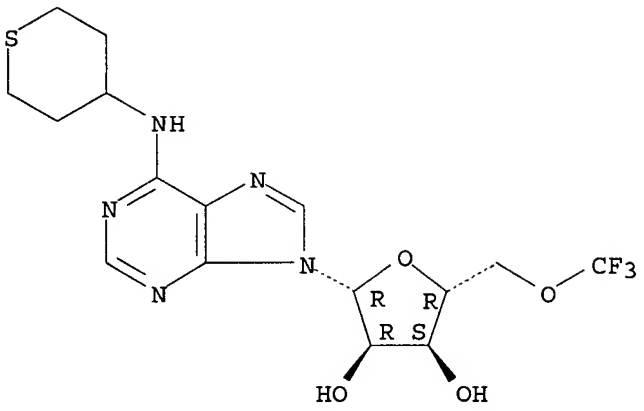
RN 223761-60-2 HCAPLUS
CN Adenosine, N-[(1S,2S)-2-fluorocyclopentyl]-5'-O-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



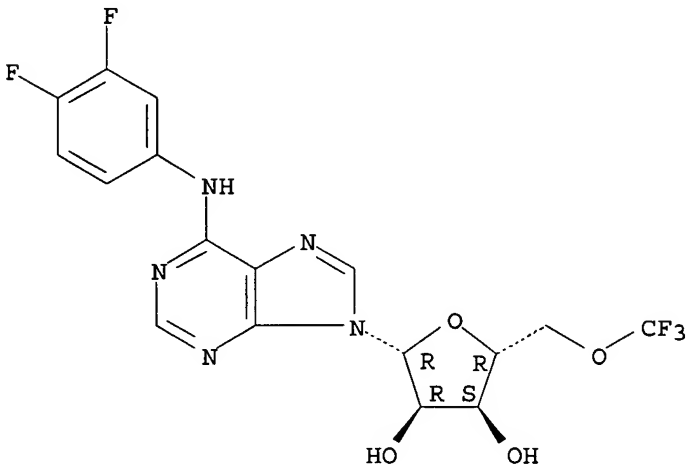
RN 223761-61-3 HCAPLUS
CN Adenosine, N-(tetrahydro-2H-thiopyran-4-yl)-5'-O-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



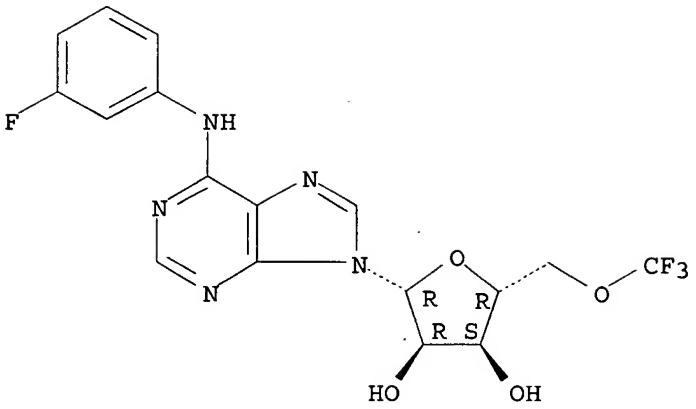
RN 223761-62-4 HCAPLUS
CN Adenosine, N-(3,4-difluorophenyl)-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



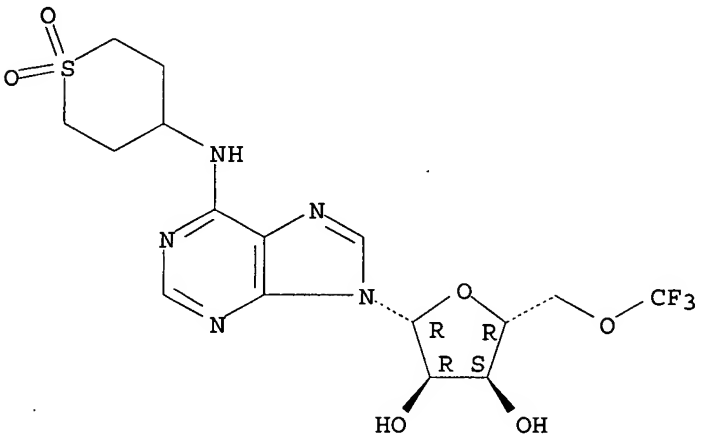
RN 223761-63-5 HCAPLUS
CN Adenosine, N-(3-fluorophenyl)-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



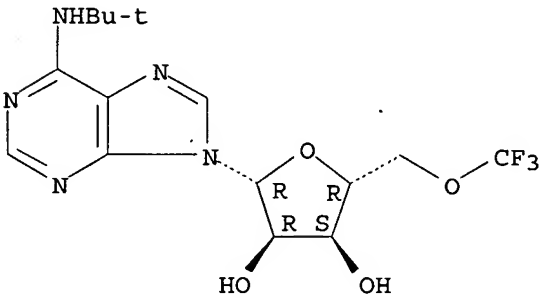
RN 223761-64-6 HCAPLUS
CN Adenosine, N-(tetrahydro-1,1-dioxido-2H-thiopyran-4-yl)-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 223761-65-7 HCAPLUS
CN Adenosine, N-(1,1-dimethylethyl)-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

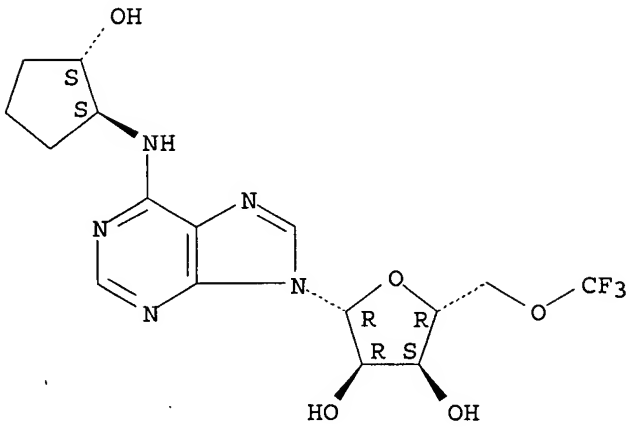
Absolute stereochemistry.



RN 223761-67-9 HCAPLUS

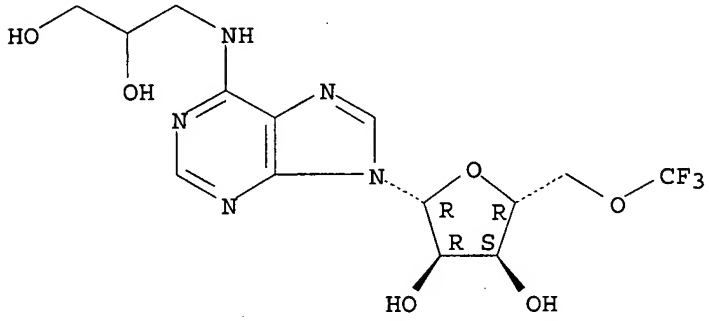
CN Adenosine, N-[(1S,2S)-2-hydroxycyclopentyl]-5'-O-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



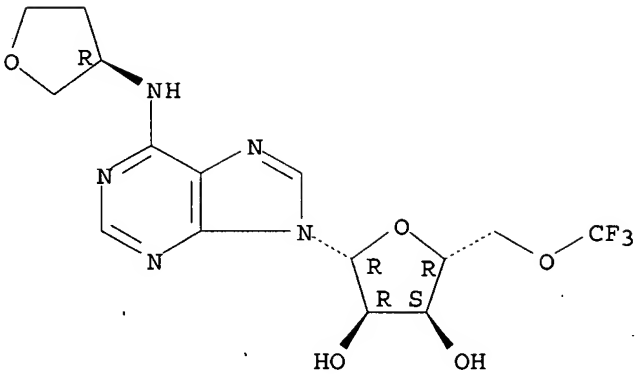
RN 223761-68-0 HCAPLUS
CN Adenosine, N-(2,3-dihydroxypropyl)-5'-O-(trifluoromethyl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



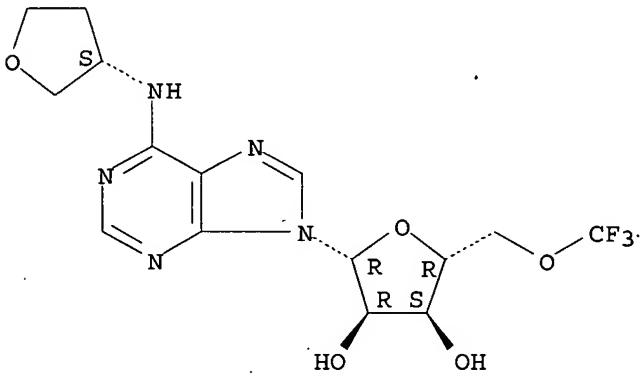
RN 223761-69-1 HCAPLUS
CN Adenosine, N-[(3R)-tetrahydro-3-furanyl]-5'-O-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



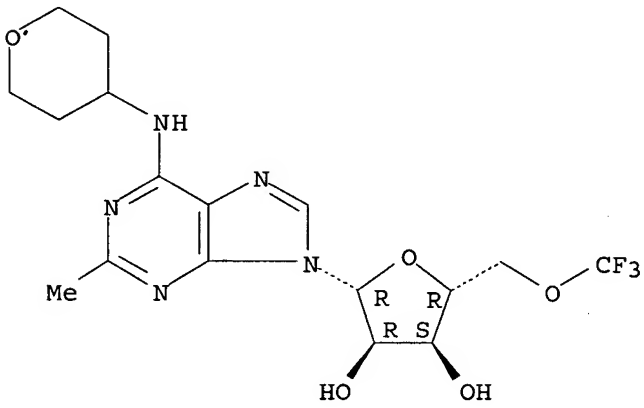
RN 223761-70-4 HCAPLUS
CN Adenosine, N-[(3S)-tetrahydro-3-furanyl]-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 223761-73-7 HCAPLUS
CN Adenosine, 2-methyl-N-(tetrahydro-2H-pyran-4-yl)-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

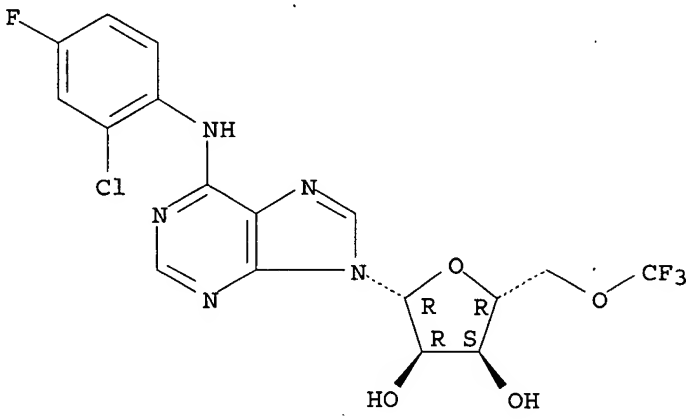
Absolute stereochemistry.



RN 223761-74-8 HCAPLUS

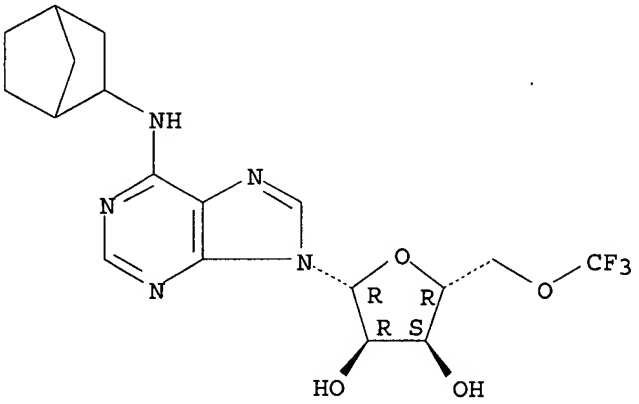
CN Adenosine, N-(2-chloro-4-fluorophenyl)-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



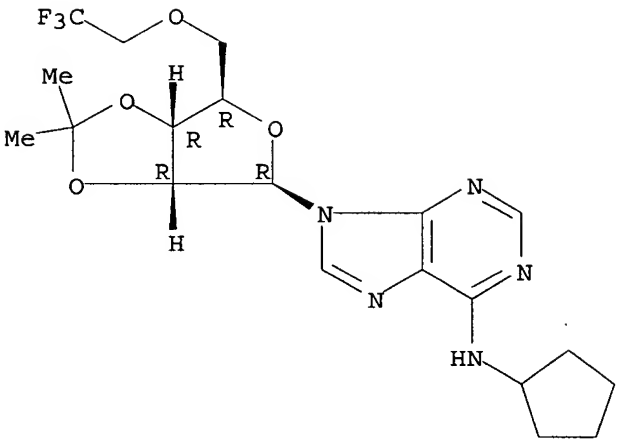
RN 223919-49-1 HCAPLUS
CN Adenosine, N-bicyclo[2.2.1]hept-2-yl-5'-O-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



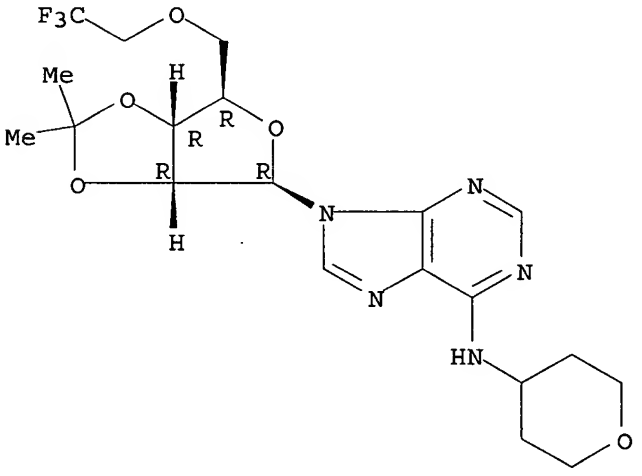
IT **223761-84-0P 223761-86-2P 223761-95-3P 223761-96-4P**
(preparation of nucleosides as adenosine A1 receptors)
RN 223761-84-0 HCAPLUS
CN Adenosine, N-cyclopentyl-2',3'-O-(1-methylethylidene)-5'-O-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



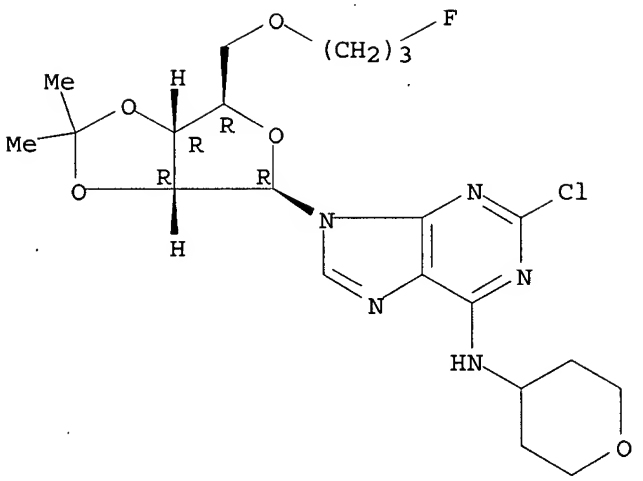
RN 223761-86-2 HCAPLUS
CN Adenosine, 2',3'-O-(1-methylethylidene)-N-(tetrahydro-2H-pyran-4-yl)-5'-O-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



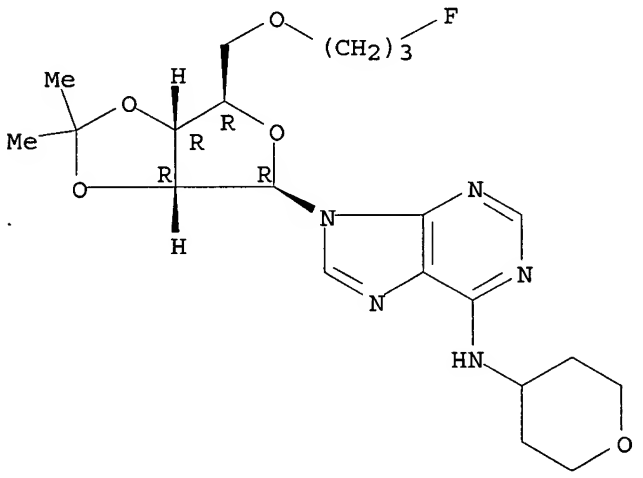
RN 223761-95-3 HCAPLUS
CN Adenosine, 2-chloro-5'-O-(3-fluoropropyl)-2',3'-O-(1-methylethylidene)-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 223761-96-4 HCAPLUS
CN Adenosine, 5'-O-(3-fluoropropyl)-2',3'-O-(1-methylethylidene)-N-(tetrahydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-00
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT **223761-50-0P 223761-51-1P** 223761-52-2P
223761-53-3P 223761-54-4P 223761-55-5P
223761-56-6P 223761-57-7P 223761-58-8P
223761-59-9P 223761-60-2P 223761-61-3P
223761-62-4P 223761-63-5P 223761-64-6P
223761-65-7P 223761-66-8P **223761-67-9P**
223761-68-0P 223761-69-1P 223761-70-4P
223761-71-5P 223761-72-6P **223761-73-7P**
223761-74-8P 223919-49-1P
(preparation of nucleosides as adenosine A1 receptors)
IT 68327-04-8P 103626-58-0P 223756-94-3P 223761-75-9P
223761-76-0P 223761-77-1P 223761-78-2P 223761-79-3P

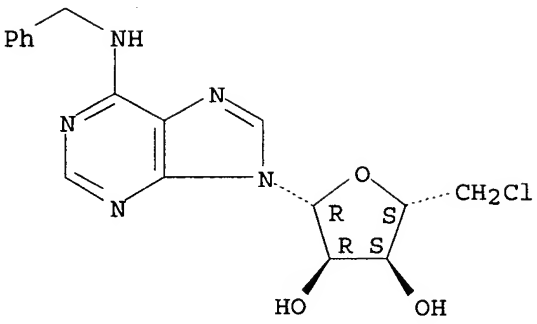
223761-80-6P 223761-81-7P 223761-82-8P 223761-83-9P
223761-84-0P 223761-85-1P **223761-86-2P**
223761-87-3P 223761-88-4P 223761-89-5P 223761-90-8P
223761-91-9P 223761-92-0P 223761-93-1P 223761-94-2P
223761-95-3P 223761-96-4P 223761-97-5P
(preparation of nucleosides as adenosine A1 receptors)

L40 ANSWER 7 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:205653 HCAPLUS
DOCUMENT NUMBER: 130:282291
TITLE: N6,5'-Disubstituted Adenosine Derivatives as Partial Agonists for the Human Adenosine A3 Receptor
AUTHOR(S): Van Tilburg, Erica W.; von Kuenzel, Jacobien; de Groote, Miriam; Vollinga, Roel C.; Lorenzen, Anna; IJzerman, Ad P.
CORPORATE SOURCE: Division of Medicinal Chemistry, Leiden/Amsterdam Center for Drug Research, Leiden, 2300 RA, Neth.
SOURCE: Journal of Medicinal Chemistry (1999), 42(8), 1393-1400
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 5'-(Alkylthio)-substituted analogs of N6-benzyl- and N6-(3-iodobenzyl)adenosine were synthesized in 37-61% overall yields. The affinities of these compds. for the adenosine A1, A2a, and A3 receptors were determined using rat brain cortex, rat brain striata, and stably transfected human A3 receptors in HEK 293 cells, resp. The compds. proved to be selective for the adenosine A3 receptor and displayed affinities in the nanomolar range. Three compds. had the highest affinities for the A3 receptor with Ki values ranging from 8.8 to 27.7 nM. In the N6-benzyl series, compound LUF 5403, with a 5'-methylthio group, maintained a reasonable affinity and had the highest selectivity for the A3 receptor. Compound LUF 5411, with an N6-(3-iodobenzyl) group and a 5'-(n-propylthio) substituent, had the highest A3 selectivity of all of the compds. and also displayed high affinity for this receptor (Ki = 44.3 nM). The compds. were also evaluated for their ability to stimulate [35S]GTPγ[S] binding in cell membranes expressing the human adenosine A3 receptor. It appeared that the N6,5'-disubstituted adenosine derivs. behaved as partial agonists. Four compds. had very high intrinsic activities; addnl., when tested in a cAMP assay, these compds. also behaved as partial agonists.

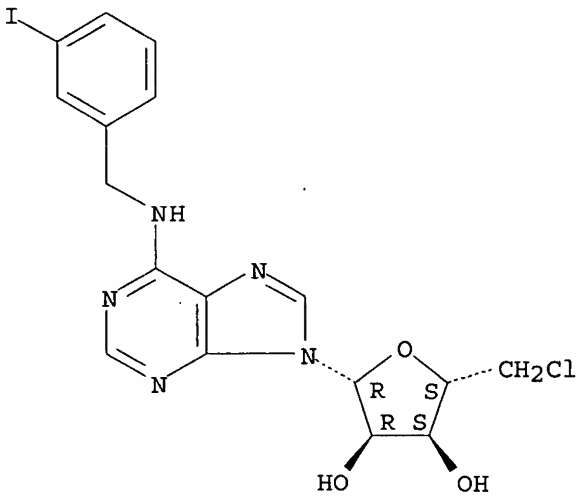
IT **111109-98-9P 222546-72-7P**
(preparation of N6,5'-disubstituted adenosine derivs. as partial agonists for the human adenosine A3 receptor)
RN 111109-98-9 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 222546-72-7 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-[(3-iodophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 4294-16-0P **111109-98-9P** 163152-30-5P
222546-72-7P
(preparation of N6,5'-disubstituted adenosine derivs. as partial agonists for the human adenosine A3 receptor)
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 8 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:171411 HCAPLUS
DOCUMENT NUMBER: 130:325325
TITLE: A convenient and practical synthesis of coenzyme B12 enriched in 13C in the cobalt-bound carbon
AUTHOR(S): Cheng, Shifa; Zang, Erle; Brown, Kenneth L.
CORPORATE SOURCE: Department of Chemistry, Xavier University of Louisiana, New Orleans, LA, 70125, USA
SOURCE: Synthetic Communications (1999), 29(5),

891-903
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:325325

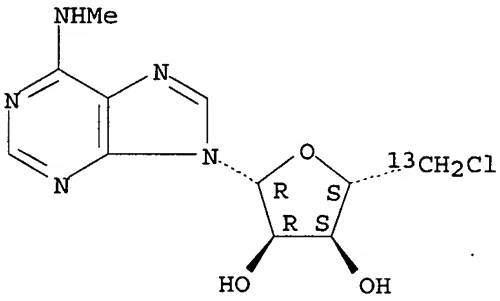
AB [A15-13C]Adenosyl-cobalamin in which the labeled carbon is bound to the cobalt atom, and its analogs were synthesized from D-[5-13C]ribose through anomeric hydroxyl activation, coupling with adenosines, and then alkylation of reduced B12. The synthetic routes described here are mild, efficient, and proceed in reasonable yield.

IT **223906-65-8P 223906-66-9P**
(preparation and reaction of in the synthesis of coenzyme B12 enriched in 13C in the cobalt-bound carbon)

RN 223906-65-8 HCAPLUS

CN Adenosine-5'-13C, 5'-chloro-5'-deoxy-N-methyl- (9CI) (CA INDEX NAME)

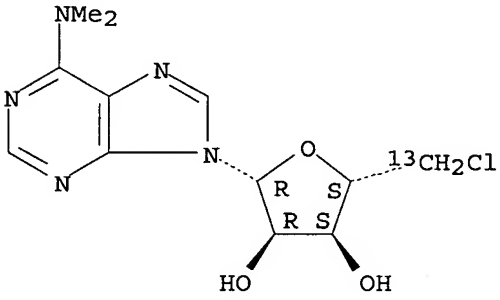
Absolute stereochemistry.



RN 223906-66-9 HCAPLUS

CN Adenosine-5'-13C, 5'-chloro-5'-deoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

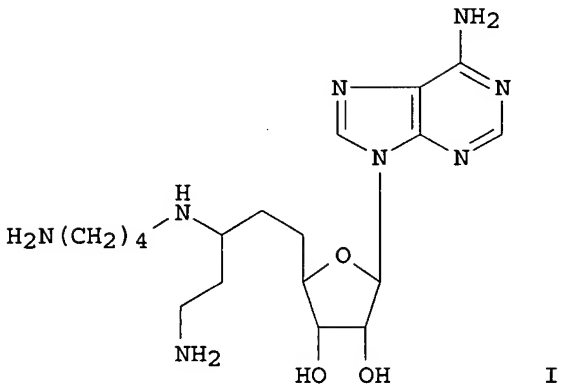


CC 33-9 (Carbohydrates)
Section cross-reference(s): 26

IT 14463-33-3P, Cob(II)alamin 54447-57-3P, Adenosine-5'-13C 54447-58-4P 184000-85-9P 223906-62-5P 223906-63-6P 223906-64-7P **223906-65-8P 223906-66-9P**
(preparation and reaction of in the synthesis of coenzyme B12 enriched in 13C in the cobalt-bound carbon)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 9 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:666993 HCAPLUS
DOCUMENT NUMBER: 123:144496
TITLE: Synthesis and Biochemical Evaluation of Adenosylspermidine, a Nucleoside-Polyamine Adduct Inhibitor of Spermidine Synthase
AUTHOR(S): Lakanen, John R.; Pegg, Anthony E.; Coward, James K.
CORPORATE SOURCE: Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109-1055, USA
SOURCE: Journal of Medicinal Chemistry (1995), 38(14), 2714-27
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:144496
GI

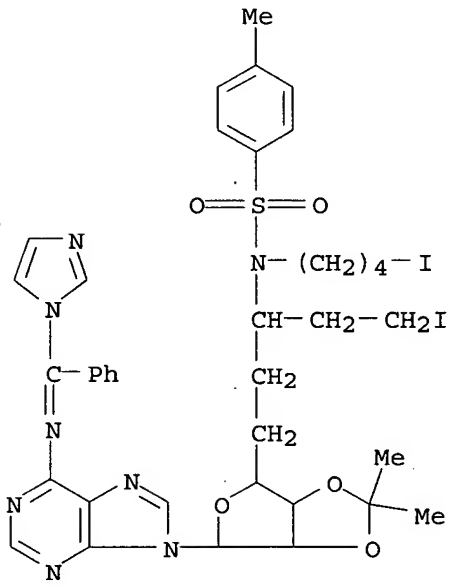


I

AB The synthesis of a new class of multi-substrate adduct inhibitors of polyamine biosynthesis has been investigated. The first target compound I, designed to inhibit spermidine synthase, was obtained and proved to be a very potent inhibitor of that enzyme. Two synthetic routes to effect the coupling of the polyamine spermidine to the nucleoside adenosine were studied. The first route involved a proposed Wittig or Julia olefination reaction to form the critical 5'-6' carbon-carbon bond between the nucleoside and polyamine moieties This route failed due to a facile β-elimination of a portion of the side chain from a carbanion intermediate during either coupling reaction. A second route involved a reductive amination approach and proved to be successful. The new inhibitor, given the trivial name adenosylspermidine, is the most potent inhibitor of spermidine synthase prepared to date.

IT **166194-10-1P**
(synthesis of adenosylspermidine as inhibitor of spermidine

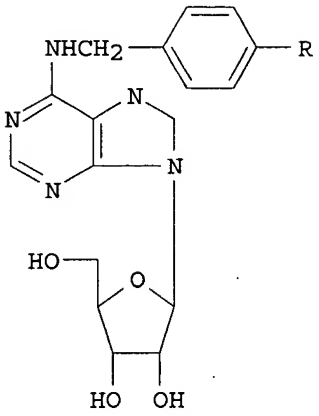
synthase)
RN 166194-10-1 HCAPLUS
CN 1H-Imidazole, 1-[[[9-[5,6,7,8,9-pentadeoxy-9-iodo-7-[(4-iodobutyl)[(4-methylphenyl)sulfonyl]amino]-2,3-O-(1-methylethylidene)-β-D-ribo-nonofuranosyl]-9H-purin-6-yl]imino]phenylmethyl]-, (7'ξ)- (9CI) (CA INDEX NAME)



CC 33-9 (Carbohydrates)
Section cross-reference(s): 7
IT 4426-52-2P 149365-02-6P 166193-85-7P 166193-86-8P
166193-87-9P 166193-88-0P 166193-89-1P 166193-90-4P
166193-91-5P 166193-92-6P 166193-93-7P 166193-94-8P
166193-95-9P 166193-96-0P 166193-97-1P 166193-98-2P
166193-99-3P 166194-00-9P 166194-01-0P 166194-02-1P
166194-04-3P 166194-05-4P 166194-06-5P 166194-07-6P
166194-08-7P 166194-09-8P **166194-10-1P** 166194-11-2P
166194-12-3P
(synthesis of adenosylspermidine as inhibitor of spermidine synthase)

L40 ANSWER 10 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:25811 HCAPLUS
DOCUMENT NUMBER: 122:133631
TITLE: Synthesis of substituted-benzyl and sugar-modified analogs of 6-N-(4-nitrobenzyl) adenosine and their interactions with "ES" nucleoside transport systems
AUTHOR(S): Robins, Morris J.; Asakura, Jun-ichi; Kaneko, Masakatsu; Shibuya, Susumu; Jakobs, Ewa S.; Agbanyo, Francisca R.; Cass, Carol E.; Paterson, Alan R. P.
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2H7, Can.
SOURCE: Nucleosides & Nucleotides (1994), 13(6-7), 1627-46
CODEN: NUNUD5; ISSN: 0732-8311

DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

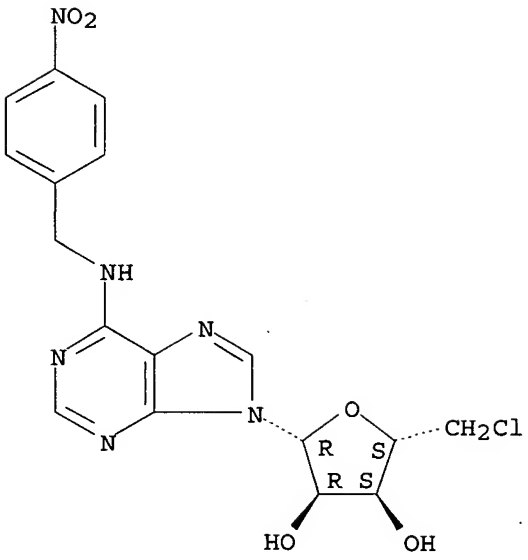
AB Four classes of 6-x-benzylated purine nucleosides, (i) 6-N-(substituted-benzyl)adenosines, (ii) 6-N-(4-nitrobenzyl) adenine nucleosides with modified sugars, (iii) 6-N(S)-(4-azidobenzyl) derivs. of adenosine, 6-thioinosine, and 6-thioguanosine, and (i.v.) 6-N-{4-N-[acyl(sulfonyl)amino]benzyl}a denosines, e.g. I (R = NO2, NH2, N3, NHAc, NHBz, NHCOCH2Cl, NHCOBu, NHCOCMe3, NHCONMe2, NHSO2Me), were synthesized and their binding interactions with "es-NT" (equilibrative, inhibitor-sensitive nucleoside transport) systems were studied. Several tight-binding analogs were found.

IT **160999-65-5P**
(preparation and antitumor activity of)

RN 160999-65-5 HCAPLUS

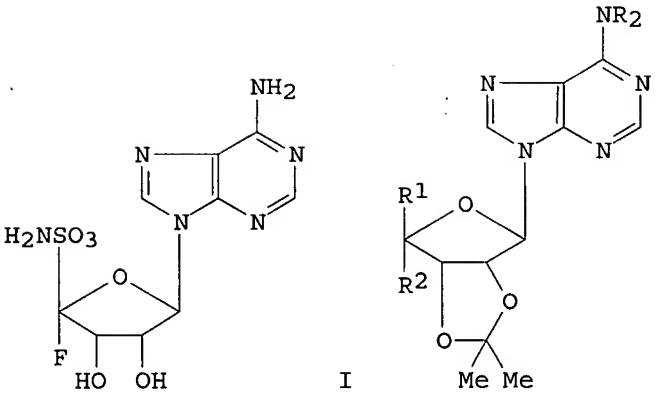
CN Adenosine, 5'-chloro-5'-deoxy-N-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 40297-54-9P 40896-41-1P 40896-45-5P 56527-33-4P
56527-35-6P 63554-95-0P 85107-83-1P 95523-13-0P
101565-95-1P 130117-68-9P 130117-69-0P 130117-70-3P
130117-71-4P 130117-72-5P 130117-73-6P 130117-74-7P
130117-75-8P 130135-62-5P 130135-63-6P 160999-57-5P
160999-58-6P 160999-59-7P 160999-60-0P 160999-61-1P
160999-62-2P 160999-63-3P 160999-64-4P **160999-65-5P**
160999-66-6P 160999-67-7P 160999-68-8P 160999-69-9P
160999-70-2P
(preparation and antitumor activity of)

L40 ANSWER 11 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:54876 HCAPLUS
DOCUMENT NUMBER: 120:54876
TITLE: Synthetic approaches towards nucleocidin and selected analogs; anti-HIV activity in 4'-fluorinated nucleoside derivatives
AUTHOR(S): Maguire, Anita R.; Meng, Wei Dong; Roberts, Stanley M.; Willetts, Andrew J.
CORPORATE SOURCE: Dep. Chem., Univ. Exeter, Exeter/Devon, EX4 4QD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (15), 1795-808
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



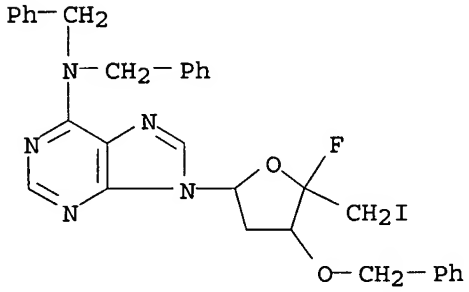
I II

AB Nucleocidin I has been synthesized from the adenosine derivative II (R = R2 = H, R1 = CH2OH) via the intermediacy of the dihalogeno compound II (R = Bz, R1 = CH2I, R2 = F). The latter compound showed slight but significant activity against HIV-infected cells while II (R = Bz, R1 = F, R2 = CH2I; R = Bz, R1 = CH2Cl, R2 = H) were inactive. Synthetic approaches towards other 4'-fluorinated nucleoside derivs. are also described.

IT **151725-79-0P 151725-80-3P**
(preparation of)

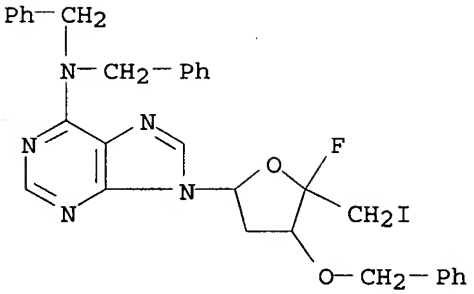
RN 151725-79-0 HCAPLUS

CN Adenosine, 2',5'-dideoxy-4'-C-fluoro-5'-iodo-N,N-bis(phenylmethyl)-3'-O-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 151725-80-3 HCAPLUS

CN 9H-Purin-6-amine, 9-[2,5-dideoxy-4-C-fluoro-5-iodo-3-O-(phenylmethyl)-α-L-threo-pentofuranosyl]-N,N-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 4099-81-4P 33962-34-4P 57731-88-1P 60102-26-3P 66792-21-0P
151725-76-7P **151725-79-0P 151725-80-3P**
151725-83-6P 151725-84-7P 151725-85-8P 151725-88-1P
151725-92-7P 151725-93-8P 151725-94-9P 151725-95-0P
(preparation of)

L40 ANSWER 12 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:497690 HCAPLUS
DOCUMENT NUMBER: 111:97690
TITLE: Preparation of N-6-aralkyladenosines having selective adenosine A2 receptor binding activity and pharmaceutical compositions containing them
INVENTOR(S): Bridges, Alexander James; Ortwine, Daniel Fred; Trivedi, Bharat Kalidas
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

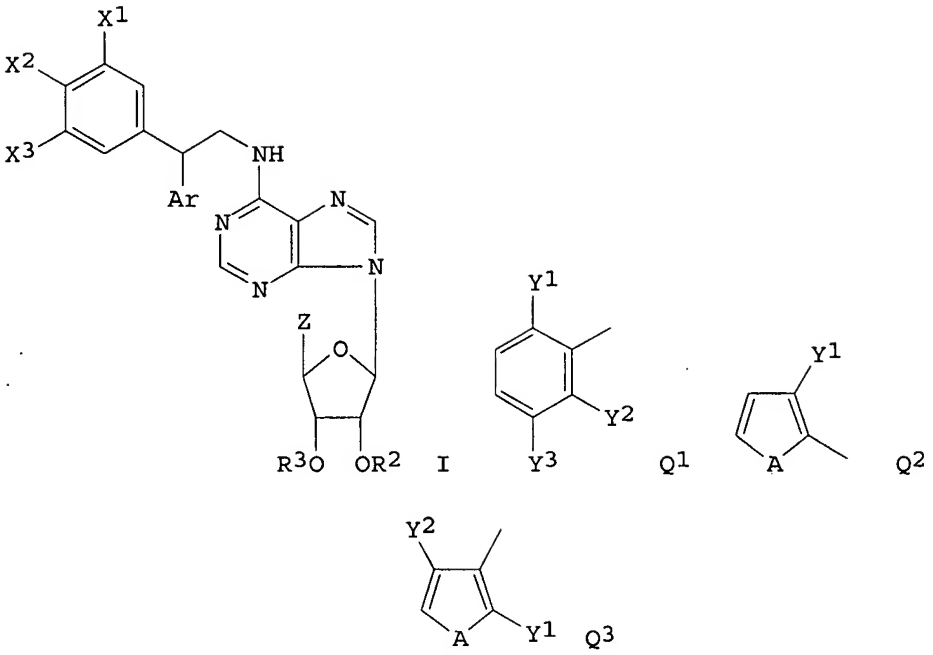
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8803147	A1	19880505	WO 1987-US2719	19871019
W: AU, BB, BG, BR, DK, FI, HU, JP, KP, KR, LK, MC, MG, MW, NO, RO, SD, SU, US, US				
RW: AT, BE, BJ, CF, CG, CH, CM, DE, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
AU 8782761	A1	19880525	AU 1987-82761	19871019
DK 8803577	A	19880629	DK 1988-3577	19880629
NO 8802887	A	19880629	NO 1988-2887	19880629
PRIORITY APPLN. INFO.:			US 1986-925185 A2	19861031

US 1987-90830 A2 19870828

WO 1987-US2719 A 19871019

OTHER SOURCE(S): MARPAT 111:97690

GI



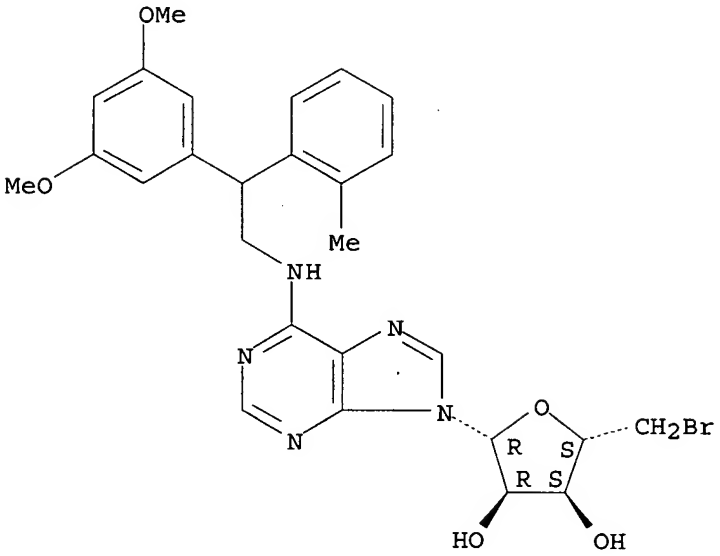
AB The title compds. [I; Ar = Q1, Q2, Q3; A = O, S; X1, X2, X3, Y1, Y2, Y3 = H, halo, alkyl, alkylthio, alkoxy, etc.; R2, R3 = H, alkanoyl, (substituted) benzoyl; or R2R3 = alkylidene; Z = (substituted) Me, dihydroxyphosphono, etc.] and their pharmaceutically acceptable acid addition salts, useful as cardiovascular agents, analgesics, antipsychotics, etc., are prepared (E)-2-(2,6-Dimethylphenyl)nitroethene (preparation given) was treated with PhMgBr in toluene at -30° and the resulting diarylnitroethene was reduced with LiAlH4 to give 2-(2,6-dimethylphenyl)-2-phenylethylamine, which was refluxed with 6-chloropurine riboside in EtOH containing Et3N for 15 h to give N-6-[2-(2,6-dimethylphenyl)-2-phenylethyl]adenosine (II). In an adenosine receptor binding study, II was > 6 times more strongly bound to A2 receptors than to A1 receptors.

IT **120355-39-7P**
(preparation of, as analgesic and cardiovascular and CNS agent)

RN 120355-39-7 HCAPLUS

CN Adenosine, 5'-bromo-5'-deoxy-N-[2-(3,5-dimethoxyphenyl)-2-(2-methylphenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-167
ICS A61K031-70
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 114675-10-4P 114675-11-5P 114675-12-6P 114675-13-7P
114675-14-8P 114675-15-9P 114675-16-0P 114675-17-1P
114675-18-2P 114691-56-4P **120355-39-7P** 120355-40-0P
120355-41-1P 120368-88-9P 120368-89-0P 120368-90-3P
120368-91-4P 120368-92-5P 120368-93-6P 120368-94-7P
120368-95-8P 120368-96-9P 120368-97-0P 120368-98-1P
120368-99-2P 120369-00-8P 120369-01-9P 120369-02-0P
120369-03-1P 120369-04-2P 120369-05-3P 120369-06-4P
120369-07-5P 120369-08-6P 120369-09-7P 120442-40-2P
(preparation of, as analgesic and cardiovascular and CNS agent)

L40 ANSWER 13 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:493537 HCAPLUS
DOCUMENT NUMBER: 109:93537
TITLE: Preparation and testing of N-[(arylcycloalkyl)methyl]adenosines as analgesics, antipsychotics, sedatives, antihypertensives, and antianginals
INVENTOR(S): Bridges, Alexander J.; Hamilton, Harriet W.; Moos, Walter H.; Szotek, Deedee L.
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: Eur. Pat. Appl., 49 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 232813	A2	19870819	EP 1987-101268	1987 0130
EP 232813	A3	19890322		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4755594	A	19880705	US 1986-936766	1986 1209
ZA 8700120	A	19880831	ZA 1987-120	1987 0108
CA 1270821	A1	19900626	CA 1987-527145	1987 0112
AU 8767972	A1	19870806	AU 1987-67972	1987 0123
AU 592728	B2	19900118		
FI 8700371	A	19870801	FI 1987-371	1987 0128
DK 8700466	A	19870801	DK 1987-466	1987 0129
NO 8700390	A	19870803	NO 1987-390	1987 0130
NO 165843	B	19910107		
NO 165843	C	19910417		
JP 62228095	A2	19871006	JP 1987-18787	1987 0130
PRIORITY APPLN. INFO.:			US 1986-825513 A	1986 0131
			US 1986-936766 A	1986 1209

OTHER SOURCE(S): CASREACT 109:93537; MARPAT 109:93537

GI For diagram(s), see printed CA Issue.

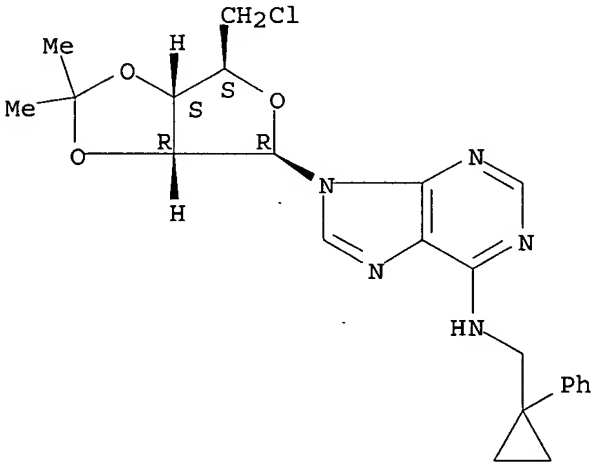
AB The title compds. [I; Ar = (substituted) Ph, naphthalenyl, thienyl, furanyl, thiazolyl, pyridyl, 2-pyrimidinyl; A = bond, O, S, CH(CH2)qMe, Me(CH2)rC(CH2)sMe; R1 = H, alkyl; G = H, alkyl, PhCH2, acyl, Bz; D = H, halo, amino, acylamino, alkylamino, cycloalkylamino; E = H, halo, amino, hydrazinyl; Z = CH2Q; Q = H, OH, halo, cyano, N3, amino, alkoxy, acyloxy, alkylthio, alkylsulfonyl, etc; m, n, q, r, s = 0-3; x = 0-2] were prepared as CNS and cardiovascular agents. 6-Chloropurine riboside, 1-phenylcyclopropanemethylamine (prepared by cyclocondensation of PhCH2CN with BrCH2CH2Br, followed by reduction), and Et2N were refluxed 2 h in EtOH to give 79% N-[(1-phenylcyclopropyl)methyl]adenosine (II). In rats 3 mg II/kg reduced blood pressure 23%. II also had an ED50 of 0.55 mg/kg in rats in a conditioned avoidance test, indicative of antipsychotic activity.

IT **115816-33-6P**
(preparation and hydrolysis of, in preparation of drug)

RN 115816-33-6 HCAPLUS

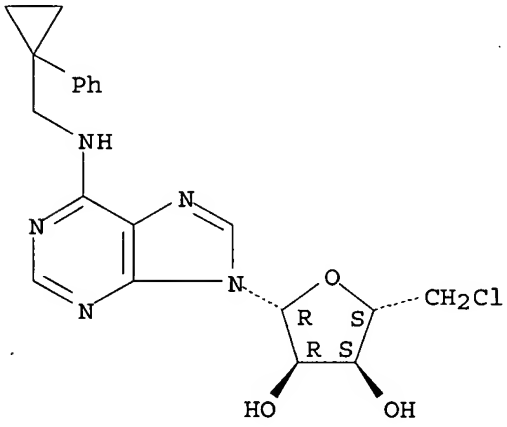
CN Adenosine, 5'-chloro-5'-deoxy-2',3'-O-(1-methylethylidene)-N-[(1-phenylcyclopropyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



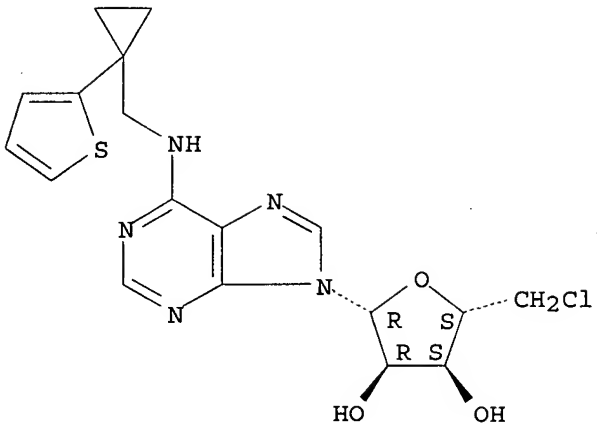
IT **115816-09-6P 115816-24-5P**
(preparation of, as CNS agent and cardiovascular agent)
RN 115816-09-6 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-[(1-phenylcyclopropyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 115816-24-5 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-[[1-(2-thienyl)cyclopropyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-167
ICS A61K031-70
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT **115816-33-6P**
(preparation and hydrolysis of, in preparation of drug)
IT 115816-07-4P 115816-08-5P **115816-09-6P** 115816-10-9P
115816-11-0P 115816-12-1P 115816-13-2P 115816-14-3P
115816-15-4P 115816-16-5P 115816-17-6P 115816-18-7P
115816-19-8P 115816-20-1P 115816-21-2P 115816-22-3P
115816-23-4P **115816-24-5P** 115816-25-6P 115816-26-7P
115816-27-8P 115816-28-9P 115816-29-0P 115816-30-3P
115842-19-8P
(preparation of, as CNS agent and cardiovascular agent)

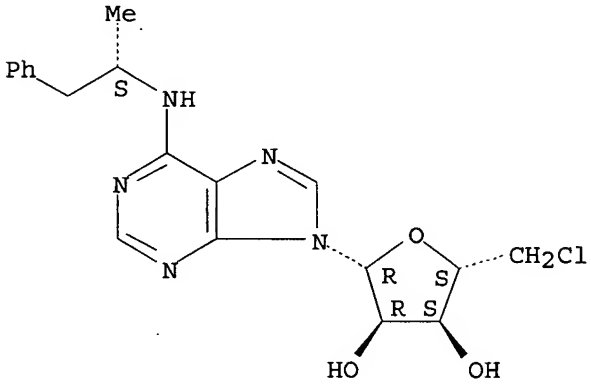
L40 ANSWER 14 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:16690 HCAPLUS
DOCUMENT NUMBER: 108:16690
TITLE: Correlation of adenosine receptor affinities and cardiovascular activity
AUTHOR(S): Hamilton, H. W.; Taylor, M. D.; Steffen, R. P.; Haleen, S. J.; Bruns, R. F.
CORPORATE SOURCE: Dep. Chem., Warner-Lambert/Parke-Davis Pharm. Res., Ann Arbor, MI, 48105, USA
SOURCE: Life Sciences (1987), 41(20), 2295-302
CODEN: LIFSAK; ISSN: 0024-3205
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Binding affinities of 28 adenosine analogs at A1 adenosine receptors [rat whole brain membranes, [3H]N6-cyclohexyladenosine (CHA)], and at A2 adenosine receptors [rat striatal membranes, 5'-N-ethylcarboxamidoadenosine (NECA) were compared to their EC25 (25% change from control) values for decreasing heart rate and increasing coronary flow in the isolated rat heart. Heart rate (an A1 response) correlated with A1 binding affinity but not with A2 binding affinity; conversely, coronary flow (an A2 response) correlated with A2 binding affinity but not with A1 binding affinity. Apparently, the brain A1 and A2 receptors, studied by binding methods, bear close similarities to their resp. counterparts in the heart, studied by means of functional responses.
IT **103626-55-7**

(adenosine receptor affinity for, in brain, cardiovascular activity in relation to)

RN 103626-55-7 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-(1-methyl-2-phenylethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2-8 (Mammalian Hormones)

IT 146-77-0 892-48-8 2457-80-9 4294-16-0 29217-90-1
35920-39-9 36396-99-3 38594-96-6 38594-97-7 41552-82-3
41552-95-8 53296-10-9 54241-03-1 75145-80-1 99798-07-9
99798-09-1 99798-11-5 101565-57-5 103450-84-6 103450-86-8
103626-55-7 103659-76-3 103791-09-9 103834-49-7
103881-79-4 107656-16-6 111864-01-8 111864-02-9
(adenosine receptor affinity for, in brain, cardiovascular activity in relation to)

L40 ANSWER 15 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:613991 HCAPLUS

DOCUMENT NUMBER: 107:213991

TITLE: Alternate substrates and inhibitors of 1-aminocyclopropane-1-carboxylic acid synthase

AUTHOR(S): Khani-Oskouee, Shahrokh; Ramalingam, Kondareddiar; Kalvin, Douglas; Woodard, Ronald W.

CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109-1065, USA

SOURCE: Bioorganic Chemistry (1987), 15(2), 92-9
CODEN: BOCMBM; ISSN: 0045-2068

DOCUMENT TYPE: Journal

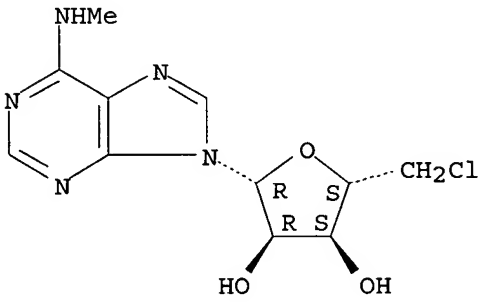
LANGUAGE: English

AB Structural analogs of (-)-S-adenosyl-L-methionine (SAM), in which the heterocyclic base was modified, were used to elucidate the active site conformation of the enzyme 1-aminocyclopropane-1-carboxylic acid (ACC) synthase, which was partially purified from Lycopersicon esculentum (tomato). These potential substrate analogs were screened for activity both as substrates and(or) as inhibitors of ACC synthase. In general, ACC synthase had a rather rigid specificity for the structural features of the natural substrate (SAM), in that only the purine base adenosine and adenosine analogs in which the N6 atom was modified were substrates.

IT **19254-36-5 59987-43-8 111109-98-9**

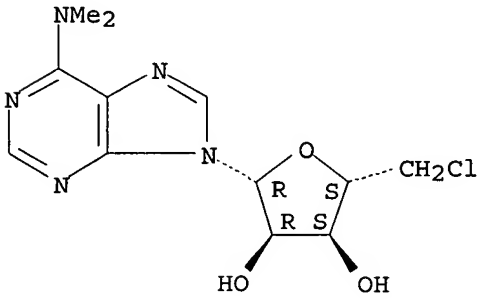
(reaction of, with homocysteine sodium salt)
RN 19254-36-5 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-methyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



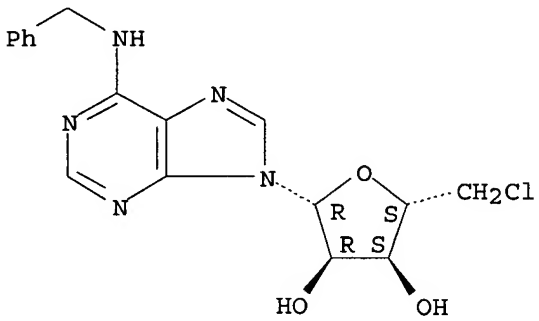
RN 59987-43-8 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 111109-98-9 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

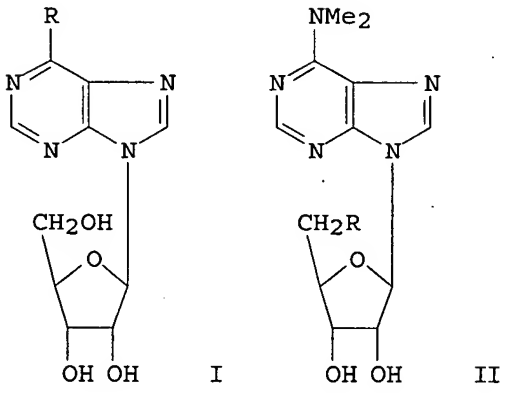
Absolute stereochemistry.



CC 7-3 (Enzymes)
IT **19254-36-5** 39947-13-2 53186-64-4 53186-65-5
59987-43-8 111109-98-9

(reaction of, with homocysteine sodium salt)

L40 ANSWER 16 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:207577 HCAPLUS
DOCUMENT NUMBER: 104:207577
TITLE: Preparation of S-(N6,N6-dimethyladenosyl)-L-methionine
AUTHOR(S): Ramalingam, Kondareddiar; Woodard, Ronald W.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109, USA
SOURCE: Carbohydrate Research (1985), 142(1), 123-6
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:207577
GI



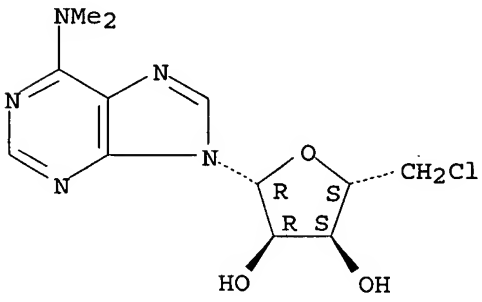
AB 6-Chloro-9-(β-D-ribofuranosyl)purine I (R = Cl) was converted into I (R = NMe2) in 92% yield which was chlorinated with SOCl2 to give 5'-chloro-5'-deoxy-N6,N6-dimethyladenosine II (R = Cl). Displacement of chloride by L-homocysteine mono-Na salt and methylation produced the sulfonium salt II [R = SMe(CH2)2CH(NH2)CO2H].

IT **59987-43-8P**
(preparation and condensation of, with L-homocysteine)

RN 59987-43-8 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

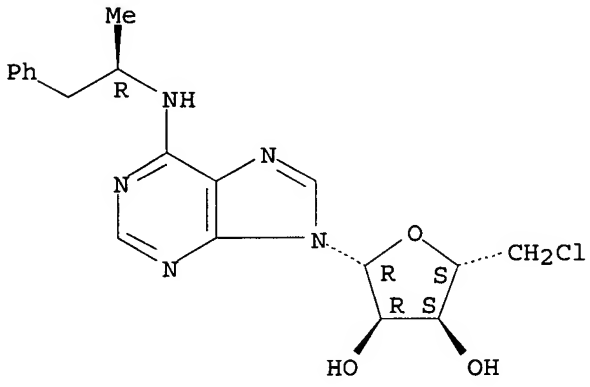
Absolute stereochemistry.



CC 33-9 (Carbohydrates)
Section cross-reference(s): 34
IT **59987-43-8P**
(preparation and condensation of, with L-homocysteine)

L40 ANSWER 17 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:88936 HCAPLUS
DOCUMENT NUMBER: 104:88936
TITLE: Ribose-modified adenosine analogs as adenosine receptor agonists
AUTHOR(S): Taylor, Michael D.; Moos, Walter H.; Hamilton, Harriet W.; Szotek, Deedee S.; Patt, William C.; Badger, Edward W.; Bristol, James A.; Bruns, Robert F.; Heffner, Thomas G.; Mertz, Thomas E.
CORPORATE SOURCE: Dep. Chem., Warner-Lambert/Parke-Davis Pharm. Res., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (1986), 29(3), 346-53
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:88936
AB Analogs of the potent adenosine receptor agonist (R)-N-(1-methyl-2-phenylethyl)adenosine (R-PIA), modified at N9, were prepared and evaluated for adenosine A1 and A2 receptor binding and in vivo central nervous system and cardiovascular effects. The modifications at N9 include deoxy sugars, 5'-substituted-5'-deoxyribose, non-ribose sugars, sugar ring homologs, and acyclic sugar analogs. Most of the derivs. have poor affinity for adenosine receptors. Only minor modifications at C5' and C3' maintain potent binding. In general, those derivs. exhibiting in vivo behavioral or cardiovascular effects also have the highest affinity for adenosine receptors.
IT **99798-10-4P**
(preparation and biol. activity of)
RN 99798-10-4 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(1-methyl-2-phenylethyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

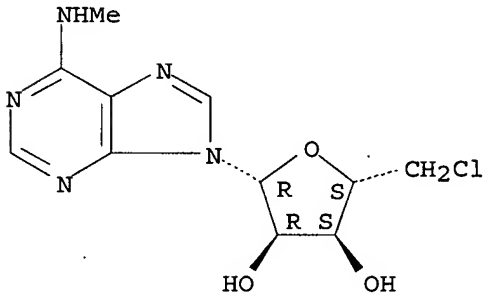


CC 33-9 (Carbohydrates)

Section cross-reference(s): 1
IT 58-61-7DP, ribose modified analogs 99797-97-4P 99797-98-5P
99797-99-6P 99798-00-2P 99798-01-3P 99798-02-4P
99798-07-9P 99798-08-0P 99798-09-1P **99798-10-4P**
99798-11-5P 99798-13-7P 99798-15-9P 99798-19-3P
99798-20-6P 99880-92-9P 99880-93-0P
(preparation and biol. activity of)

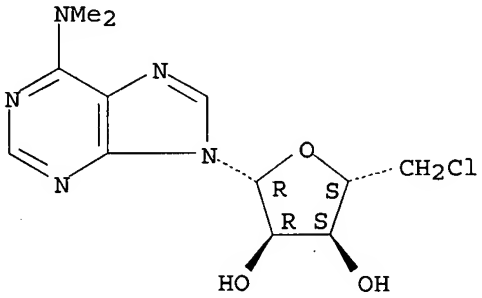
L40 ANSWER 18 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:139584 HCAPLUS
DOCUMENT NUMBER: 100:139584
TITLE: An improved synthesis of S-adenosylhomocysteine and related compounds
AUTHOR(S): Ramalingam, Kondareddiar; Woodard, Ronald W.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109, USA
SOURCE: Journal of Organic Chemistry (1984), 49(7), 1291-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB S-Adenosylhomocysteine (SAH) analogs were prepared in 45-80% yields via the reaction of the appropriate 5'-chloro-5'-deoxynucleoside and the Na salt of homocysteine in water. The method allows not only for the first successful synthesis of N6,N6-dimethyladenosyl-L-homocysteine but the yields of the SAH analogs are consistently higher (5-30%) and the initial products are purer than with previous methods.
IT **19254-36-5 59987-43-8**
(reaction of, with homocysteine sodium salt)
RN 19254-36-5 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-methyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



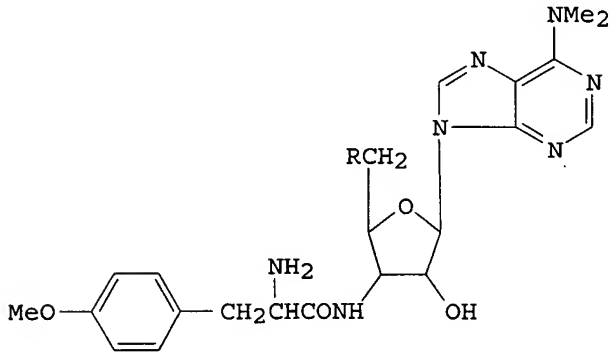
RN 59987-43-8 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 33
IT 892-48-8 **19254-36-5** 31652-78-5 **59987-43-8**
(reaction of, with homocysteine sodium salt)

L40 ANSWER 19 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:45905 HCAPLUS
DOCUMENT NUMBER: 96:45905
TITLE: 5'-Chloropuromycin. Inhibition of protein synthesis and antitrypanosomal activity
AUTHOR(S): Vince, Robert; Lee, Heejoo; Narang, A. S.; Shirota, Frances N.
CORPORATE SOURCE: Coll. Pharm., Univ. Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Journal of Medicinal Chemistry (1981), 24(12), 1511-14
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I, R=Cl
II, R=H

AB I [80362-00-1] and II [43157-40-0], puromycin derivs., were synthesized and tested for their ability to inhibit protein formation in vitro and for their antitrypanosomal activity in mice. Both I and II inhibited protein formation by acting as substrates at the peptidyltransferase site of ribosomes, whereas only I exhibited significant antitrypanosomal activity in mice . In rats, the aminonucleosides released by the in vivo hydrolysis of I and II exhibited no nephrotoxicity, whereas the corresponding

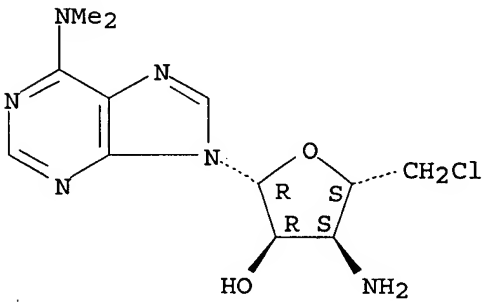
aminoglycoside of puromycin caused severe nephrotoxic manifestations.

IT **80361-98-4P**
(preparation and nephrotoxicity of)

RN 80361-98-4 HCAPLUS

CN Adenosine, 3'-amino-5'-chloro-3',5'-dideoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-5 (Pharmacology)
Section cross-reference(s): 28

IT 43157-41-1P **80361-98-4P**
(preparation and nephrotoxicity of)

L40 ANSWER 20 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:524330 HCAPLUS

DOCUMENT NUMBER: 85:124330

TITLE: New syntheses of S-adenosylhomocysteine and S-adenosylmethionine analogs

AUTHOR(S): Legraverend, M.; Michelot, R.

CORPORATE SOURCE: Inst. Chim. Subst. Nat., Gif-sur-Yvette, Fr.

SOURCE: Biochimie (1976), 58(6), 723-9
CODEN: BICMBE; ISSN: 0300-9084

DOCUMENT TYPE: Journal

LANGUAGE: French

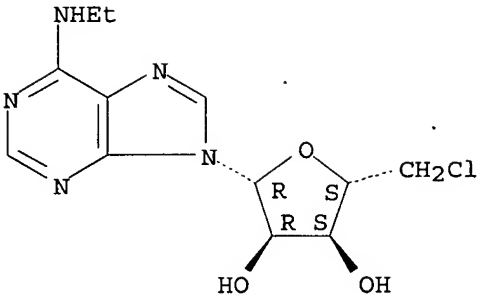
AB Analogs of S-adenosyl homocysteine and S-adenosyl methionine, potential inhibitors of methyl-transferases, were prepared in which either the amino-acid chain is replaced by various aliphatic radicals or the N-6 amino group of adenine is substituted.

IT **19254-38-7P 59987-43-8P 60406-43-1P**
(preparation and reaction with sulfur containing amino acids)

RN 19254-38-7 HCAPLUS

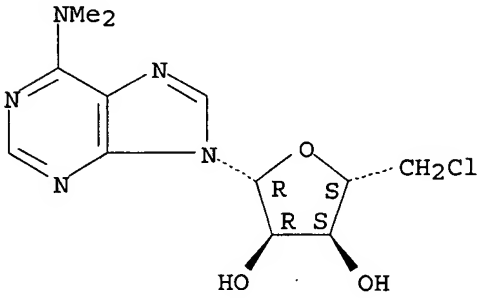
CN Adenosine, 5'-chloro-5'-deoxy-N-ethyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



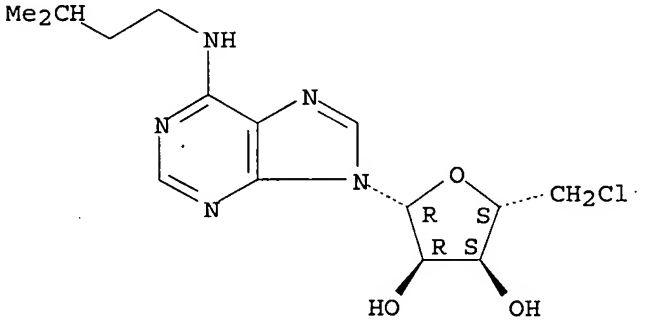
RN 59987-43-8 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 60406-43-1 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-(3-methylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-2 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 33
IT **19254-38-7P 59987-43-8P 60406-43-1P**
(preparation and reaction with sulfur containing amino acids)

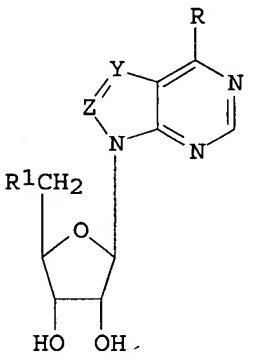
L40 ANSWER 21 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:487098 HCAPLUS
DOCUMENT NUMBER: 85:87098

TITLE: Potential inhibitors of S-adenosylmethionine-dependent methyltransferases. 4. Further modifications of the amino acid and base portions of S-adenosyl-L-homocysteine

AUTHOR(S): Borchardt, R. T.; Huber, J. A.; Wu, Yih Shiong
CORPORATE SOURCE: Dep. Biochem., Univ. Kansas, Lawrence, KS, USA

SOURCE: Journal of Medicinal Chemistry (1976), 19(9), 1094-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

II, R=NH_2, R^1=$SCH_2CH_2CH(NH_2)CO_2H$, Y=Z=N

III, R=NHMe, R^1=$SCH_2CH_2CH(NH_2)CO_2H$, Y=N, Z=CH

IV, R=NH_2, R^1=$SCH_2CH_2CH(NH_2)CO_2H$, Y=Z=CH

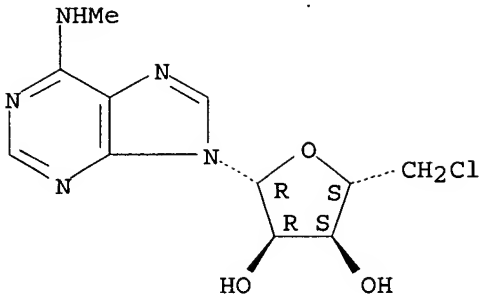
AB Five structural analogs (I) of S-adenosyl-L-homocysteine (L-SAH) [979-92-0] were prepared and evaluated for inhibition of the transmethylations catalyzed by catechol O-methyltransferase (EC 2.1.1.6) [9012-25-3], phenylethanolamine N-methyltransferase (EC 2.1.1.28) [9037-68-7], histamine N-methyltransferase (EC 2.1.1.8) [9029-80-5], hydroxyindole O-methyltransferase (EC 2.1.1.4) (HIOMT) [9029-77-0], and indoleethylamine N-methyltransferase (INMT) [9073-61-4]. S-8-azaadenosyl-L-homocysteine [59987-42-7] is a potent and selective inhibitor of HIOMT. Consistent with previous studies of N6-methyl-3-deazaadenosyl-L-homocysteine [53199-58-9], S-N6-methyladenosyl-L-homocysteine (III) [53228-06-1] is a very potent, selective inhibitor of INMT. S-tubercidinyl-L-homocysteine (IV) [57344-98-6] is a fairly potent, but nonselective inhibitor of all the methyltransferases studied. Structure requirements for binding of L-SAH to methyltransferases and design of analogs as specific enzyme inhibitors is discussed.

IT **19254-36-5P 59987-43-8P**
(preparation and condensation with homocysteine)

RN 19254-36-5 HCAPLUS

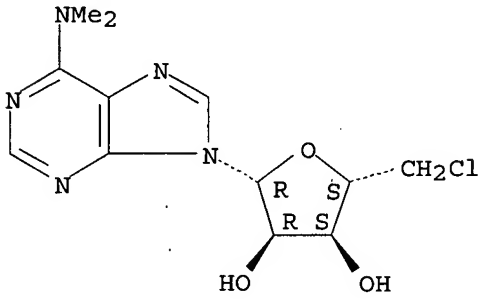
CN Adenosine, 5'-chloro-5'-deoxy-N-methyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 59987-43-8 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

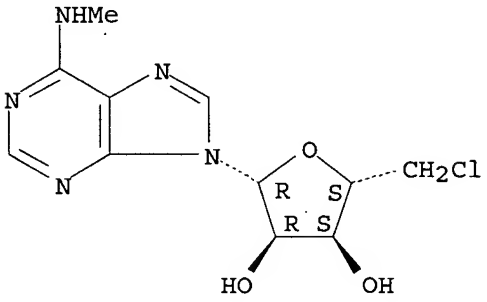


CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 33, 7
IT **19254-36-5P** 53458-85-8P **59987-43-8P**
(preparation and condensation with homocysteine)

L40 ANSWER 22 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:90472 HCAPLUS
DOCUMENT NUMBER: 84:90472
TITLE: Convenient preparation of S-adenosylhomocysteine and related compounds
AUTHOR(S): Borchardt, Ronald T.; Huber, Joan A.; Wu, Yih Shiong
CORPORATE SOURCE: Dep. Biochem., Univ. Kansas, Lawrence, KS, USA
SOURCE: Journal of Organic Chemistry (1976), 41(3), 565-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compds. (I, R = adenine, N6-methyladenine, N6-methyl-3-deazaadenine, 7-deazaadenine residue, R1 = R2 = OH; R = adenine, R1 = OH; R2 = H; R1 = H, R2 = OH) were prepared in 45-75% yields by condensation of the appropriate 5'-chloro-5'-deoxynucleosides with L-homocystine in Na and liquid NH3. The 5'-chloro-5'-deoxynucleosides were prepared in 75-100% yield from the corresponding nucleosides using SOCl2 in P(O)(NMe2)3.
IT **19254-36-5P**
(preparation and reaction with homocysteine)

RN 19254-36-5 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-methyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-7 (Carbohydrates)
Section cross-reference(s): 34, 28
IT 892-48-8P **19254-36-5P** 53458-85-8P 57274-13-2P
57274-14-3P 57274-15-4P
(preparation and reaction with homocysteine)

L40 ANSWER 23 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:78563 HCAPLUS
DOCUMENT NUMBER: 68:78563
TITLE: Disubstituted adenosine derivatives
PATENT ASSIGNEE(S): Boehringer, C. F., und Soehne G.m.b.H.
SOURCE: Brit., 4 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1101108		19680131	GB 1966-53974	1966 1202
DE 1545645			DE	
FR 1503243			FR	
US 3475408		19691028	US	1966 1116

PRIORITY APPLN. INFO.: DE 1965 1206

GI For diagram(s), see printed CA Issue.
AB The preparation of disubstituted adenosine derivs. I by N-alkylation or N-alkenylation followed by acid hydrolysis was described. Thus, 5'-chloro-N6-formyl-2',3'-O-isopropylidenadenosine, prepared from 5 g. N6-formyl-2',3'-O-isopropylidene-5'-O-p-tolylsulfonyladenosine, was dissolved in 50 ml. HCONMe2, stirred 18 hrs. with 25 g. BaO, 0.7 g. Ba(OH)2.8H2O, and 12 ml. PrI, mixed with 100 ml. CHCl3, and centrifuged. The organic phase was shaken

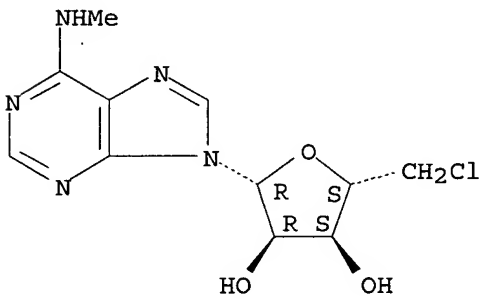
with aqueous S2O32- solution, evaporated, and saponified with dilute HCO2H to give
28% I (R = Pr, R' = Cl), m. 104-8°. Similarly prepared were I (R = Pr, R' = azido), m. 112-13°, I (R = Bu, R' = Cl), m. 90-3°, and I (R = hexyl, R' = Cl), m. 78-70°. A slurry of 10 g. 2',3'-O-isopropylidenadenosine in 100 ml. HCONMe2 and 30 ml. allyl iodide was stirred 5 hrs., kept 8 hrs., decolorized with concentrated NaHSO3, boiled 25 min. with 100 ml. 2N NaOH, and extracted with CHCl3. The extract was evaporated to leave a syrup which was dissolved in 60 ml. pyridine, cooled to -20°, mixed with 10 g. p-ClO2SC6H4Me, kept 18 hrs. at -20°, diluted with water, and extracted with CHCL3 to give 14 g. crude N6-allyl-2',3'-O-isopropylidene-5'-O-p-tolylsulfonyladenosine (II) which was dissolved in 85 ml. of a mixture containing equivalent amts. of HCO2H and Ac2O, kept 1 day at room temperature, and evaporated in vacuo. The residue was dissolved in 100 ml. Me2SO, heated 20 min. on a steam bath with 9 g. LiCl, mixed with water, and extracted with CHCl3. The residue after evaporation was dissolved in 50 ml. HCO2H, water was added to cloudiness, and the mixture was kept 4 days and neutralized with aqueous NH3 to give 35% I (R = allyl, R' = Cl), m. 143-6°. Similarly prepared were I (R = Et, R' = Cl), m. 153-5°, and I (R = iso-Bu, R' = Cl), m. 70°. A solution of crude II in 100 ml. Me2SO was heated 15 min. on a steam bath with 9 g. NaN3 and treated as above to give 20% I (R = allyl, R' = azido), m. 90-2°. Crude II was added in portions to a solution of NaSMe, prepared from 1.4 g. Na and 3 g. MeSH, in 100 ml. liquid NH3 and the mixture was stirred 4 hrs., stripped of NH3, mixed with 1 g. NH4Cl, and extracted with CHCl3. The extract was saponified with N H2SO4 to give 40% I (R = allyl, R' = MeS). Similarly prepared was I (R = Me, R' = MeS), m. 173-5°. These compds. dilate peripheral blood vessels of the circulatory system and suppress cardiac activity.

IT **19254-36-5P 19254-37-6P 19254-38-7P 19254-39-8P 19280-33-2P 19280-34-3P 19361-48-9P 19372-13-5P**
(preparation of)

RN 19254-36-5 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-methyl- (8CI, 9CI) (CA INDEX NAME)

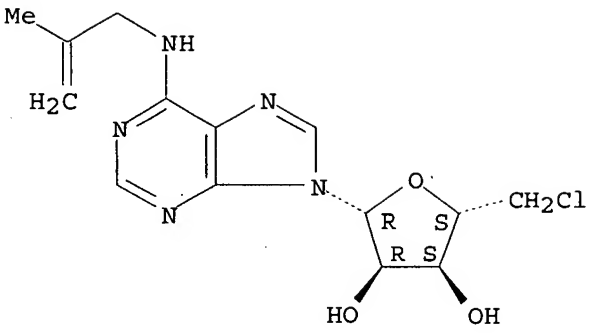
Absolute stereochemistry.



RN 19254-37-6 HCAPLUS

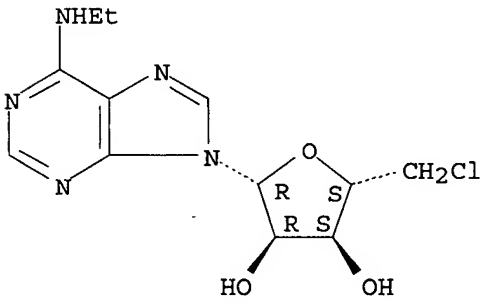
CN Adenosine, 5'-chloro-5'-deoxy-N-(2-methylallyl)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



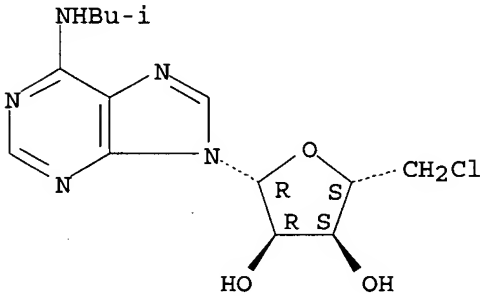
RN 19254-38-7 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-ethyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



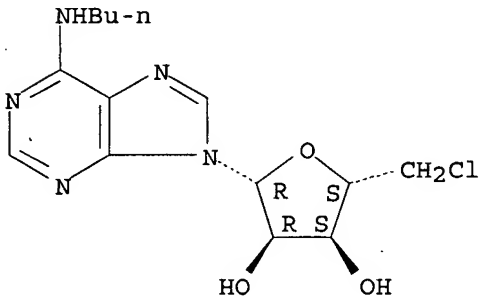
RN 19254-39-8 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-isobutyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



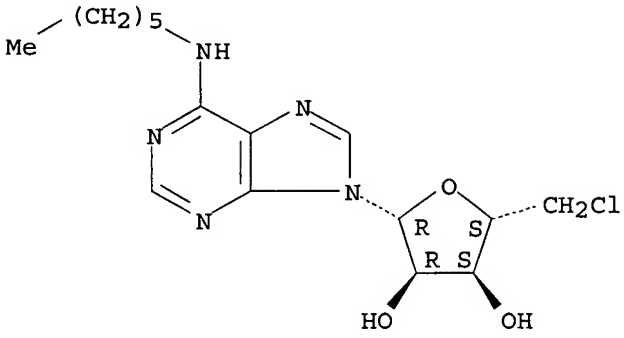
RN 19280-33-2 HCAPLUS
CN Adenosine, N-butyl-5'-chloro-5'-deoxy- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



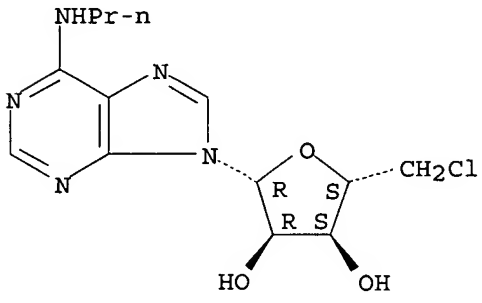
RN 19280-34-3 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-hexyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



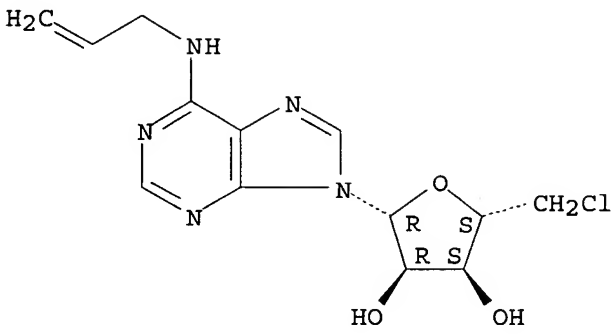
RN 19361-48-9 HCAPLUS
CN Adenosine, 5'-chloro-5'-deoxy-N-propyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 19372-13-5 HCAPLUS
CN Adenosine, N-allyl-5'-chloro-5'-deoxy- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



IC C07D
CC 33 (Carbohydrates)
IT 19254-35-4P **19254-36-5P** **19254-37-6P**
19254-38-7P **19254-39-8P** 19254-40-1P
19254-41-2P **19280-33-2P** **19280-34-3P**
19361-48-9P **19372-13-5P** 19422-86-7P
(preparation of)